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IMPROVING THE DEPICTION OF UNCERTAINTY IN SIMULATION MODELS BY EXPLOITING THE POTENTIAL OF GAUSSIAN QUADRATURES

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Related publications

Parts of this thesis are submitted to peer-reviewed international journals for publication, are published as scientific reports, or are presented at international scientific conferences. They contain co-authorships. These papers are listed below with references to specific sections of this thesis:

Journal submissions:

1. Stepanyan, Davit; Grethe, Harald; Zimmermann, Georg; Siddig, Khalid; Deppermann, Andre; Feuerbacher, Arndt; Luckmann, Jonas; Valin, Hugo; Nishizawa, Takamasa; Ermolieva, Tatiana; Havlik, Petr (2021): Multiple rotations of Gaussian quadratures: an efficient method for uncertainty analyses in large-scale simulation models. In *Environmental Modelling & Software*, 136. DOI: 10.1016/j.envsoft.2020.104929.
   Chapter 3
2. Stepanyan, Davit; Zimmermann, Georg; Grethe, Harald (2020): Stochastic simulation with informed rotations of Gaussian quadratures. In *Economic Systems Research*. Under review.
   Chapter 4

Scientific reports

3. Stepanyan, Davit (2018). Application of Gaussian Quadratures in the Global Biosphere Management Model (GLOBIOM) as an Efficient Approach to Uncertainty Analysis. International Institute for Applied Systems Analysis (IIASA), Laxenburg, Austria. Available online at: http://www.iiasa.ac.at/web/home/education/yssp/YSSP_report_Davit_Stepanyan.pdf
   Chapter 3, Sections 3.4.1; 3.4.2; 3.5.2; parts of 3.6

Conference papers:

4. Stepanyan, Davit, Harald Grethe, Georg Zimmermann, Khalid Siddig, Andre Deppermann, Arndt Feuerbacher, Jonas Luckmann, Hugo Valin, Takamasa Nishizawa, Tatiana Ermolieva, and Petr Havlik (2019). Multiple Rotations of Gaussian Quadratures : An Efficient Method for Uncertainty Analyses in Large-Scale Simulation Models. Presented at the 22nd Annual Conference on Global Economic Analysis, Warsaw, Poland. Available online at: https://www.gtap.agecon.purdue.edu/resources/download/9432.pdf.
   Chapter 3

5. Stepanyan, Davit, Khalid Siddig, Harald Grethe, and Georg Zimmermann (2018). Remarks on uncertainty analysis in large-scale simulation models. Presented at the International Conference on Economic Modeling (EcoMod 2018), Venice, Italy. Available online at: https://editorialexpress.com/cgi-bin/conference/download.cgi?db_name=ECOMOD2018&paper_id=110
   Chapter 3, Sections 3.4.1; 3.4.2; 3.5.3; parts of 3.6

Declaration of own contribution

Davit Stepanyan is the lead author of the above-listed publications which evolved under his coordination. Concepts were mainly developed by him and were discussed with the co-authors. Model adaptations and simulations were done by Davit Stepanyan. The entire work has been supervised by Harald Grethe and Georg Zimmermann. Georg Zimmermann contributed strongly to understanding the mathematical concept of quadratures. The generated programming models were implemented in Wolfram Mathematica by Georg Zimmermann. Interpretation of the results, reasoning, and compiling the manuscript were done by Davit Stepanyan and were intensively discussed with co-authors.

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List of abbreviations

CES	Constant Elasticity of Substitution
CDF	Cumulative Density Function
CGE	Computable General Equilibrium
CV	Coefficient of Variation
EE	Elementary Effects (method)
ESIM	European Simulation Model
EU	European Union
FAST	Fourier Amplitude Sensitivity Test
GLOBIOM	Global Biosphere Management Model
GQ	Gaussian Quadrature
GTAP	Global Trade Analysis Project (Model)
IRGQ	Informed Rotations of Gaussian Quadratures
LES	Linear Expenditure System
LHS	Latin Hypercube Sampling
LP	Linear Programming
MC	Monte Carlo
MRGQ	Multiple Rotations of Gaussian Quadratures
PE	Partial Equilibrium
ROW	Rest of the World
SA	Sensitivity Analysis
SAM	Social Accounting Matrix
SPAM	Spatial Production Allocation Model
SSA	Systematic Sensitivity Analysis
STAGE	Static Applied General Equilibrium (Model)
TFP	Total Factor Productivity
UA	Uncertainty Analysis

Abstract

Simulation models are an established tool for assessing the impacts of exogenous shocks in complex systems. Recent increases in available computational power and speed have led to simulation models with increased levels of detail and complexity. However, this trend has raised concerns regarding the uncertainty of such model results and therefore motivated many users of simulation models to consider uncertainty in their simulations. One way is to integrate stochastic elements into the model equations, thus turning the model into a problem of (multiple) numerical integration. As, in most cases, such problems do not have analytical solutions, numerical approximation methods are applied.

The uncertainty quantification techniques currently used in simulation models are either computational expensive (Monte Carlo [MC]-based methods) or produce results of varying quality (Gaussian quadratures [GQs]). The MC-based methods are easy to apply and very effective; however, they are inefficient. For example, Haber (1970) claims that to obtain an accuracy level below 1% using the MC method, the number of iterations should range from 40,000 to 100,000. Using this many iterations is not feasible for large-scale simulation models. Hence, many researchers applying such methods in an uncertainty analysis must compromise between computational efforts and the quality of the approximations. In contrast, GQs require a minimal number of iterations (2n, where n is the number of stochastic variables) to reproduce the second central moments of a joint probability distribution. Artavia et al. (2015) found that, depending on the rotation of Stroud's octahedron, the generated GQs produce approximations of varying quality. Moreover, Villoria and Preckel (2017) compared the results approximated by GQs and the MC method for the global trade analysis

project (GTAP) model and discovered large inaccuracies in the results obtained by the GQs.

Considering the importance of efficient uncertainty quantification methods in the era of big data, this thesis aims to develop methods that decrease the approximation errors of GQs and make these methods accessible to the wider research community. For this purpose, two novel uncertainty quantification methods are developed and integrated into four different large-scale partial and general equilibrium models addressing agro-environmental issues.

Following the classification of uncertainty by its nature and source of origin in Chapter 2, Chapters 3 and 4 address the primary and secondary research objectives of this thesis.

The first novel method developed in this thesis is presented in Chapter 3. The developed method is tested in three large-scale simulation models: a comparative-static, single-country computable general equilibrium (CGE) model (McDonald and Thierfelder 2015), a global partial equilibrium (PE) model known as GLOBIOM (Havlík et al. 2011; Havlík et al. 2014), and a multi-sector recursive-dynamic CGE model (Diao and Thurlow 2012). To evaluate the quality of the results approximated by the proposed methods, benchmark results are generated using an MC-based method called the Latin hypercube sampling (LHS) method. The proposed method, named multiple rotations of Gaussian quadratures (MRGQ), reduces the approximation errors by a factor of nine using only 3.4% of the computational effort required by the MC-based methods in the most computationally demanding model. It does so by increasing the number of quadrature points slightly. In this chapter, a programming model is provided that generates MRGQ points for stochastic analysis when supplied with the necessary input data.

In Chapter 4, an important factor influencing the quality of approximations obtained by GQs is revealed. In addition, the second novel method developed in this thesis is presented. The method is tested in three large-scale simulation models, *i.e.*, a global PE model called ESIM (Grethe 2012), a global PE model known as GLOBIOM (Havlík et al. 2011; Havlík et al. 2014), and a multi-sector recursive-dynamic CGE model (Diao and Thurlow 2012). The results are evaluated against the benchmarks generated using the LHS method. The proposed method is named informed rotations of Gaussian quadratures (IRGQ) and can distinguish the rotations of Stroud's octahedron generated by the permutations of the n coordinates that produce better-quality results. The advantage of the IRGQ method over the MRGQ method is that the IRGQ method produces good quality results by preserving the original number of iterations required by the GQ method (*i.e.*, 2n, whereas the MRGQ method increases the number of iterations). These two methods can complement each other in achieving high-quality approximations and avoiding outliers. To encourage the wider research community to apply the developed methods, an LP model is also provided that produces IRGQ points or, as explained above, combines the IRGQ and MRGQ methods to achieve higher precision in the results.

This thesis provides method developments and is of high relevance for applied simulation modelers who struggle to apply computationally burdensome stochastic modeling methods. Although the methods are developed and tested in large-scale simulation models addressing agricultural issues, they are not restricted to a model type or field of application.

Keywords: Stochastic modeling, uncertainty analysis, PE model, CGE model, Gaussian quadratures, Monte Carlo sampling, efficient methods

Zusammenfassung

Simulationsmodelle sind ein etabliertes Instrument zur Analyse von Auswirkungen exogener Schocks in komplexen Systemen. Die in jüngster Zeit gestiegene verfügbare Rechenleistung und -geschwindigkeit hat die Entwicklung detaillierterer und komplexerer Simulationsmodelle befördert. Dieser Trend hat jedoch Bedenken hinsichtlich der Unsicherheit solcher Modellergebnisse aufgeworfen und daher viele Nutzer von Simulationsmodellen dazu motiviert, Unsicherheiten in ihren Simulationen zu integrieren. Eine Möglichkeit dies systematisch zu tun besteht darin, stochastische Elemente in die Modellgleichungen zu integrieren, wodurch das jeweilige Modell zu einem Problem (mehrfacher) numerischer Integrationen wird. Da es für solche Probleme meist keine analytischen Lösungen gibt, werden numerische Approximationsmethoden genutzt.

Die derzeit zur Quantifizierung von Unsicherheiten in Simulationsmodellen genutzt en Techniken, sind entweder rechenaufwändig (Monte Carlo [MC] -basierte Methoden) oder liefern Ergebnisse von heterogener Qualität (Gauß-Quadraturen [GQs]). MC-basierte Ansätze sind zwar leicht anzuwenden und sehr effektiv, jedoch ineffizient. Beispielsweise behauptet Haber (1970), dass zwischen 40.000 und 100.000 Iterationen benötigt werden würden, um mit der MC-Methode einen Genauigkeitsgrad von unter 1% zu erreichen. Eine solch hohe Zahl an Iterationen ist für große Simulationsmodelle nicht realisierbar. Daher müssen Forscher, die solche Methoden der Unsicherheitsanalyse anwenden, Kompromisse zwischen dem Rechenaufwand und der Qualität der Näherungswerte finden. Im Gegensatz dazu benötigen GQs nur eine minimale Anzahl von Iterationen (2n, wobei n die Anzahl der stochastischen Variablen ist), um die zweiten zentralen Momente einer gemeinsamen

Wahrscheinlichkeitsverteilung zu reproduzieren. Artavia et al. (2015) fanden heraus, dass die erzeugten GQs je nach Rotation des Stroudschen Oktaeders Näherungswerte von heterogener Qualität erzeugen. Darüber hinaus verglichen Villoria und Preckel (2017) die durch GQs approximierten Ergebnisse mit der MC-Methode für das Modell des Global Trade Analysis Projects (GTAP) und stellten große Ungenauigkeiten in den mit den GQs erzielten Ergebnissen fest.

In Anbetracht der Bedeutung von effizienten Methoden zur Quantifizierung von Unsicherheit im Zeitalter von „big data“ ist es das Ziel dieser Doktorthesis, Methoden zu entwickeln, die die Näherungsfehler von GQs verringern und diese Methoden einer breiteren Forschungsgemeinschaft zugänglich machen. Zu diesem Zweck werden zwei neuartige Methoden zur Quantifizierung von Unsicherheiten entwickelt und in vier verschiedene, große partielle und allgemeine Gleichgewichtsmodelle integriert, die sich mit Agrarumweltfragen befassen.

Im Anschluss an die Klassifikation von Unsicherheiten nach ihrer Art und Herkunft in Kapitel 2 befassen sich die Kapitel 3 und 4 mit den primären und sekundären Forschungszielen dieser Arbeit.

Die erste in dieser Arbeit entwickelte neuartige Methode, die in Kapitel 3 vorgestellt wird, wird in drei großen Simulationsmodellen getestet: einem komparativ-statischen, Allgemeinen Gleichgewichtsmodell (CGE) für ein Einzelland (McDonald und Thierfelder 2015), einem globalen Partiellen Gleichgewichtsmodell (PE), bekannt als GLOBIOM (Havlík et al. 2011; Havlík et al. 2014), und einem multisektoriellen rekursiv-dynamischen CGE-Modell (Diao und Thurlow 2012). Um die Qualität der durch die vorgeschlagenen Methoden approximierten Ergebnisse zu bewerten, werden Benchmark-Ergebnisse mit Hilfe einer MC-basierten Methode, des sogenannten Latin

Hypercube Samplings (LHS), generiert. Die vorgeschlagene neue Methode, die als Multiple Rotationen von Gauß-Quadraturen (MRGQ) bezeichnet wird, reduziert die Näherungsfehler um den Faktor neun und benötigt im rechenintensivsten Modell nur 3,4% der Rechenleistung, die die MC-basierten Methode erfordert, wobei die Anzahl der Quadraturpunkte nur leicht erhöht wird. In diesem Kapitel wird darüber hinaus ein lineares Optimierungsmodell (LP)-Modell vorgelegt, mit dessen Hilfe aus erforderlichen Eingabedaten MRGQ-Punkte für die stochastische Analyse erzeugt werden können.

In Kapitel 4 wird ein wichtiger Faktor aufgezeigt, der die Qualität der durch GQs erzielten Näherungen beeinflusst. Darüber hinaus wird die zweite neuartige Methode vorgestellt, die in dieser Arbeit entwickelt wurde. Auch diese Methode wird in drei großen Simulationsmodellen getestet: in einem globalen PE-Modell namens ESIM (Grethe 2012), einem globalen PE-Modell namens GLOBIOM (Havlík et al. 2011; Havlík et al. 2014) und einem multisektoriellen rekursiv-dynamischen CGE-Modell (Diao und Thurlow 2012). Die Ergebnisse werden mit mittels der LHS-Methode generierten Benchmarks verglichen und evaluiert. Die vorgeschlagene Methode wird als informierte Rotationen von Gauß-Quadraturen (IRGQ) bezeichnet und kann jene durch Permutationen der n-Koordinaten erzeugten Rotationen des Stroudschen Oktaeders erkennen, die qualitativ bessere Ergebnisse liefern. Der Vorteil der IRGQ-Methode gegenüber der MRGQ-Methode besteht darin, dass die IRGQ-Methode qualitativ gute Ergebnisse liefert, wobei sie die ursprüngliche Anzahl der Iterationen, die für die GQ-Methode erforderlich ist, beibehält (d.h. 2n, während die MRGQ-Methode die Anzahl der Iterationen erhöht). Diese beiden Methoden können sich gegenseitig ergänzen, um Näherungen von hoher Qualität zu erzeugen und Ausreißer zu vermeiden. Um die breitere Forschungsgemeinschaft zur Anwendung der

entwickelten Methoden zu ermutigen, wird ein LP-Modell vorgestellt, das IRGQ-Punkte erzeugt oder, wie oben erläutert, die IRGQ- und die MRGQ-Methode kombiniert, um eine höhere Präzision der Ergebnisse zu erreichen.

Diese Arbeit liefert methodische Entwicklungen und ist von hoher Relevanz für angewandte Simulationsmodellierer, die Schwierigkeiten bei der Anwendung von rechenintensiven stochastischen Modellierungsmethoden haben. Obwohl die Methoden in großen Simulationsmodellen für Agrarumweltfragen entwickelt und getestet werden, sind sie nicht durch Modelltyp oder Anwendungsgebiet beschränkt, sondern können ebenso in anderen Zusammenhängen angewandt werden.

Schlüsselwörter: Stochastische Modellierung, Unsicherheitsanalyse, PE-Modell, CGE-Modell, Gauß-Quadraturen, Monte-Carlo-Stichproben, effiziente Methoden

CHAPTER 1

Introduction

Chapter 1

1. Introduction

1.1. Background

> *Chance, or probability, is no longer a convenient way of accepting ignorance, but rather part of a new, extended rationality.*
>
> *Ilya Prigogine (1997), p. 155*

Simulation modeling has become increasingly popular in many areas of research. In the agro-environmental sciences, the rapid increase in available computational power and speed has led to the expansion of simulation model detail and complexity. This expansion has also increased the uncertainty associated with modeling results. To address model uncertainty, researchers usually apply different uncertainty analysis techniques via stochastic modeling, which has become a standard modeling practice. Nevertheless, the conventional methods used in uncertainty analysis are either computationally demanding or produce results of varying quality.

The incorporation of stochastic elements into a simulation model turns it into a problem of (multiple) numerical integration. Such problems cannot be solved analytically because they are not given in a closed form (Arndt et al. 2015). Instead, numerical approximation methods must be used. Haber (1970) divides numerical integration methods into two groups: probabilistic methods, which include the Monte Carlo (MC)-based methods, and efficient methods, which include the methods based on Gaussian quadratures (GQs).

Although the probabilistic methods are very effective and straightforward, such methods suffer from poor computational efficiency and require high computational efforts (Razavi and Gupta 2016). When applying such methods in simulation modeling,

it is important to conduct convergence evaluations to determine the appropriate sample size for the (quasi-) random draws from a pre-specified probability distribution (Yang 2011). However, it is not uncommon for researchers applying stochastic simulation models in the agro-environmental field to select an *ad hoc* and relatively small sample size that fits the available computational capacities, thus limiting the approximation quality (e.g., Valin et al. 2015; OECD/FAO 2017; Villoria and Preckel 2017; Mary et al. 2018). Many well-established applied simulation models used to address agro-environmental issues use one of this group's methods to conduct uncertainty analyses. For example, the global biosphere management model, also known as GLOBIOM (Havlík et al. 2011; Havlík et al. 2014), uses the MC method (Valin et al. 2015). However, there have been some recent attempts to incorporate more efficient methods into GLOBIOM, such as Stepanyan (2018). Furthermore, the Aglink-Cosimo model (Araujo-Enciso et al. 2017) uses an MC-based method called Latin hypercube sampling (LHS) (Pieralli et al. 2020).

In contrast, GQs, which are efficient methods, require a minimal amount of points to reproduce the second central moments of a joint probability distribution (Stroud 1957). This method has increasingly gained the attention of applied modelers due to its efficiency. GQ is the standard stochastic modeling approach used in the global trade analysis project (GTAP) model (Arndt 1996) and the European simulation model (ESIM) (Grethe 2012).

1.2. Terminology

Stochastic simulation modeling is relatively new to the agro-environmental sciences. Therefore, the terminology is often contradictory and lacking in uniformity. To avoid confusion, the main terminology used in this thesis is elaborated below.

Aleatory uncertainty results from the inherent randomness or natural variability in the system being analyzed (Skinner et al. 2014). Examples of this type of uncertainty include climate variability, crop yield variability, and water availability.

Complete stochastic analysis quantifies the uncertainties stemming from all the possible sources of uncertainty present in the model.

Efficiency of a method is usually assessed via the number of iterations required to obtain statistically robust results (Razavi and Gupta 2016).

Epistemic uncertainty is caused by limited knowledge of the system. In contrast to aleatory uncertainty, epistemic uncertainty can be reduced through additional research (Ascough et al. 2008).

Partial stochastic analysis quantifies uncertainties stemming from only some of the sources of uncertainty present in the model. In this thesis, partial stochastic analysis is referred to as stochastic analysis.

Robustness is defined as the stability of the results. The lower variability in the results obtained by solving a model with a sample of parameter values drawn from a probability distribution indicates a higher degree of robustness (Sheikholeslami et al. 2019).

Sensitivity analysis aims to describe the impact of modest changes in input factors on model output. It explains the changes in model output for relatively small and arbitrarily selected sets of input factors (Loucks and van Beek 2017). Figure 1.1 provides a graphical example of a sensitivity analysis.

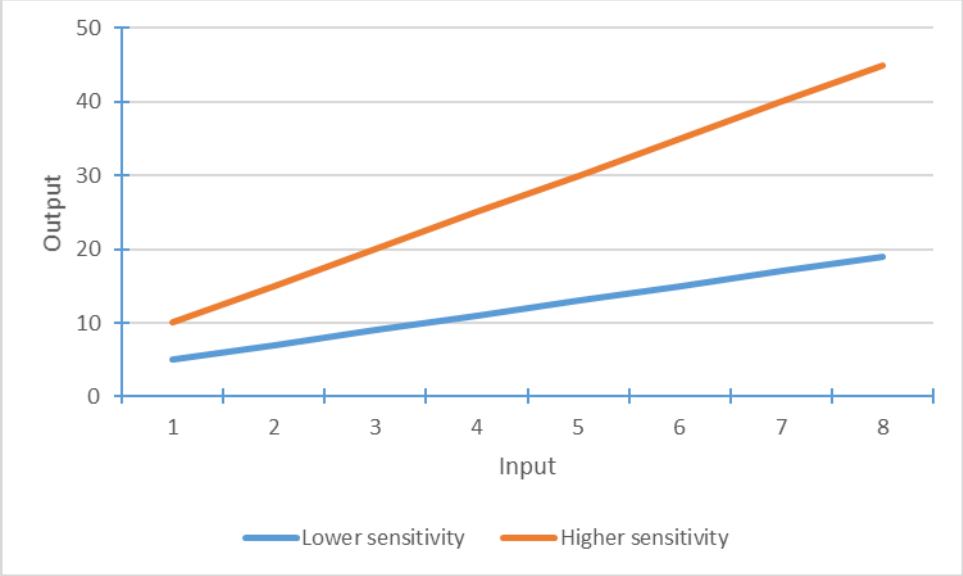

Figure 1.1. An example of a sensitivity analysis concerning changes in a model input factor.
Source: author

Stochastic variable/parameter. When a variable or parameter is sampled from a probability distribution, it is referred to as stochastic.

Systematic sensitivity analysis assumes a distribution for the input factor of interest instead of measuring the responsiveness of the model output to a small set of point estimates of input factors (Arndt 1996). Consequently, the output is also a distribution; thus, this type of analysis provides a much more comprehensive picture of the model's robustness. Systematic sensitivity analysis aims at quantifying epistemic uncertainty. An example is provided in Figure 1.2.

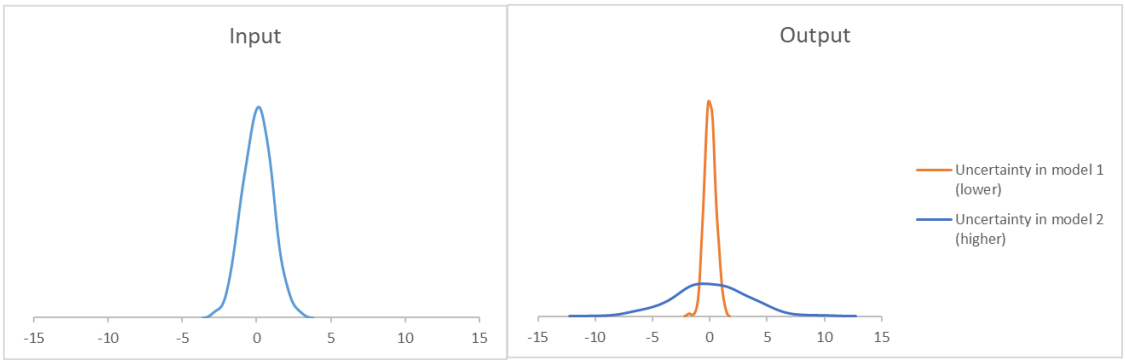

Figure 1.2. An example of systematic sensitivity analysis.
Source: author

Uncertainty is a lack of knowledge, regardless of its cause (Uusitalo et al. 2015).

Uncertainty analysis attempts to explain the entire set of possible outcomes with respect to the uncertainties inherent in the input variables, such as the weather, by describing these variables with probability distributions and producing distributions of the model outputs under input uncertainty. The difference between systematic sensitivity analysis and uncertainty analysis is that the second type of analysis generates a probability distribution based on the available historical data and considers the observed uncertainty inherent in the input factors. In contrast, the first type of analysis simply assumes a probability distribution, for example, by specifying the upper and lower values of the input factor. Uncertainty analysis aims at quantifying aleatory uncertainty.

1.3. Problem statement

Once Arndt (1996) introduced Stroud's (1957) order 3 GQ for the GTAP model, it became the standard method for conducting systematic sensitivity/uncertainty analyses in the stochastic version of the model. However, Artavia et al. (2015) discovered that the GQ method produces results of varying quality depending on the chosen rotation of Stroud's octahedron, which is used to generate the GQ points by testing eight different rotations in the ESIM model. Later, Villoria and Preckel (2017) compared the results approximated by the GQ method with the ones obtained with the MC method using the GTAP model. They discovered large deviations in the first three central moments of the results. These results led them to suggest that the computational requirements of the probabilistic approaches of stochastic modeling should be accepted and that use of the GQ method should be curtailed to avoid poor quality results. These two studies demonstrated that the results approximated by the GQ method can sometimes be of very poor quality. However, they failed to explain the factors affecting the quality of the results approximated by the GQ method and did not propose approaches for improving its quality.

1.4. Research objectives

The primary objectives of this thesis are:

1. To develop a method that reduces the approximation error in the GQ method to the level that would allow its application in large-scale simulation models without concerns regarding the quality of the approximated results.
2. To determine the factors influencing the quality of the approximations obtained by certain rotations of Stroud's octahedron.

The secondary objectives of this thesis are:

3. To confirm, in a more comprehensive framework, the findings of Artavia et al. (2015) that the quality of the approximations produced by the GQ method is indeed influenced by the rotations of Stroud's octahedron.

4. To incorporate and test the GQ-based methods in other well-established, large-scale simulation models addressing agro-environmental issues.

5. To demonstrate the computational efforts required to obtain reliable results when applying probabilistic methods of stochastic analysis in large-scale simulation models.

After Artavia et al.'s (2015) finding that the quality of the results approximated by the GQ method depends on the chosen rotation of Stroud's octahedron, the researchers applying this method faced the dilemma of whether to continue using this computationally efficient method or to simply accept the computational efforts imposed by the probabilistic methods. For example, Villoria and Preckel (2017) suggest avoiding the GQ method in favor of the MC method, given the fast growth in computational capacities. At this point, the way forward was unclear for two reasons. First, prior to this finding, the opinion that the rotations of Stroud's octahedron did not impact the quality of the GQ method prevailed (Preckel et al. 2011). Second, there was no clear understanding of the factors influencing the quality of the results obtained by certain rotations. Thus, to overcome the issue of poor approximations produced by the GQ method and to address the first research objective of this thesis, a novel approach is designed to reduce the approximation errors of the GQ method named multiple rotations of Gaussian quadratures (MRGQ). This method is successfully tested in three

very different large-scale simulation models to avoid dependence on a certain model type or data structure. The method is presented in Chapter 3.

While addressing this study's first research objective, we tested a large number of random rotations in three different large-scale simulation models. An interesting pattern was observed in the results obtained from these simulation models. We realized that certain GQ families in which the quadrature points are located far from each other (*i.e.*, they have a larger dispersion) produce relatively better-quality results than those having points located closer to each other. This observation led us to develop another novel method capable of selecting rotations that produce better quality results. The developed method is named informed rotations of Gaussian quadratures (IRGQ) and is presented in Chapter 4. The proposed method is tested using the same model and data structure as Artavia et al. (2015). To avoid dependence on one specific model type, the method is also tested in two other large-scale simulation models.

Artavia et al. (2015) tested eight arbitrarily chosen rotations in the ESIM model and concluded that the rotations influence the quality of the approximations. This finding was controversial because, up to this point, the prevailing opinion was that the opposite was true (Preckel et al. 2011). Thus, to obtain firm evidence of this claim, several GQ families generated from random rotations of Stroud's octahedron are tested in three different large-scale models. Artavia et al.'s (2015) claim is confirmed through the empirical evidence gathered via extensive computations. These results are presented in Chapter 3.

An important objective of this study is also to make other research communities using large-scale simulation models aware of these alternative and efficient stochastic modeling techniques. For this purpose, the methods developed here are incorporated

into and tested in three other simulation models that had not been exposed to efficient stochastic modeling methods prior to this investigation. These models are the GLOBIOM (Havlík et al. 2011; Havlík et al. 2014), a multi-sector recursive-dynamic CGE model (Diao and Thurlow 2012), and a single-country CGE model based on the static applied general equilibrium (STAGE) model (McDonald and Thierfelder 2015).

This study's final objective is to demonstrate the process and the computational efforts required for generating reliable benchmarks for large-scale simulation models using a probabilistic approach. For this purpose, the LHS method (Helton and Davis 2003) is used. These benchmarks are presented in Chapter 3 to evaluate the quality of the novel methods produced in this study.

1.5. Contributions to science

This study's contribution is mainly methodological, and the results will be of great interest to applied modelers. In this study, two novel, noncompetitive (*i.e.*, supplemental) methods for stochastic modeling are developed.

The first method, MRGQ, reduces the approximation error of the standard GQ method considerably while keeping the number of required iterations in an acceptable range.

The second method, IRGQ, identifies GQ families that produce better-quality results, reducing the number of iterations needed compared to the MRGQ method.

In addition to these methodological contributions, we have also developed and made publicly available programming models that provided the necessary input data generate MRGQ or IRGQ points. The generated points can be applied to any simulation model for stochastic analysis.

1.6. Outline of the thesis

Following the general introduction, terminology, and research objectives presented above, this thesis is organized as follows.

Chapter 2 provides a comprehensive classification of uncertainty based on the nature and source of the origin.

Chapter 3 presents a novel method for uncertainty analysis via MRGQ, which reduces the approximation error in the GQ method. A detailed literature review on the available uncertainty analysis methods for simulation models is also presented in this chapter, revealing their shortcomings and potential research gaps. In addition, the theoretical background for Stroud's order 3 GQ is presented in detail. A programming model is also presented that, once it is provided with the necessary input data, generates MRGQ points. These points can be implemented in other models as well.

Chapter 4 explains a factor influencing the quality of the approximations obtained by specific rotations of Stroud's octahedron. The second novel method developed in this study, IRGQ, is presented in this chapter. An LP model that generates IRGQ points is constructed and made publicly available.

Finally, Chapter 5 summarizes the key findings, highlights the limitations of this thesis, and discusses the potential for future research.

CHAPTER 2

Uncertainty classification

Chapter 2

2. Uncertainty classification

Uncertainty classifications vary considerably, depending on the context and scope (Uusitalo et al. 2015). Such differences usually cause confusion, especially among researchers from different disciplines. In this chapter, a classification of uncertainties based on their nature and source of origin is presented. Figure 2.1 displays different uncertainty categories.

Based on the nature of the uncertainty, three broad categories can be distinguished: aleatory uncertainty, epistemic uncertainty, and linguistic uncertainty (Uusitalo et al. 2015). These categories are further divided into multiple subcategories according to the source of uncertainty.

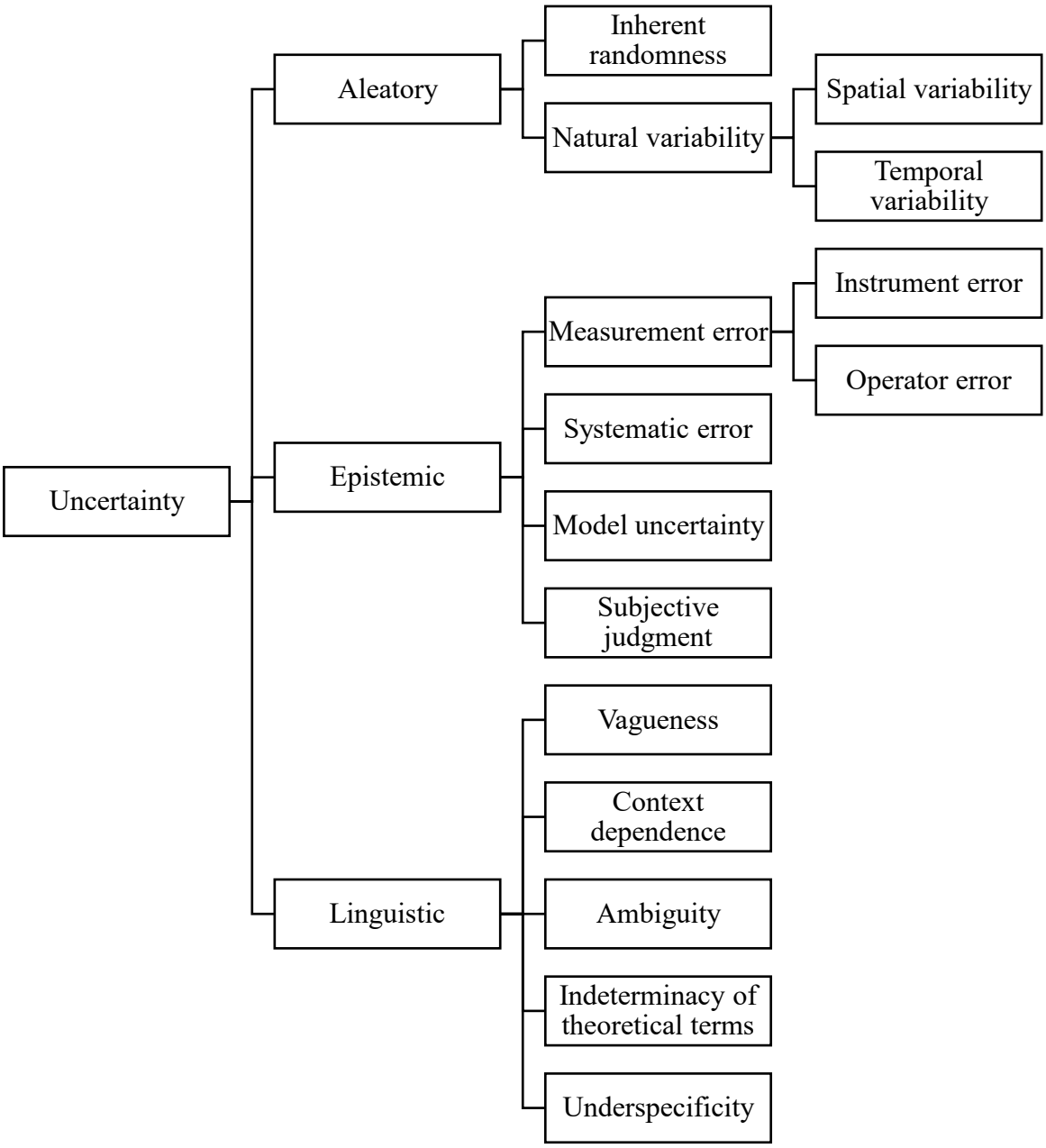

Figure 2.1. Classification of uncertainty types according to their nature and origin.

Source: author

2.1. Aleatory uncertainty

Aleatory uncertainty results from the inherent randomness or natural variability in the system being analyzed (Skinner et al. 2014). Examples of such uncertainty include climate variability, crop yield variability, and water availability. This type of uncertainty is irreducible, although additional research can lead to a better understanding of its impact on the system of interest (Refsgaard et al. 2007). Aleatory uncertainty can be quantified via uncertainty analysis techniques.

Inherent randomness

Independent of how well one knows the process and how much information one can obtain about the system, the outcome of the process cannot be calculated with certainty if inherent randomness is present in the system (Uusitalo et al. 2015). According to Regan et al. (2002), inherent randomness is introduced because the system itself is irreducible to determinism. Some well known examples of ihnerent randomness are coin tosses or the throwing of dice.

Natural variability

Complex systems usually vary through time (temporal variability) and space (spatial variability); thus, the parameters used in the model must do so as well. Therefore, no matter how many resources are devoted to measuring and estimating the parameters, there will always be a degree of uncertainty associated with them (Uusitalo et al. 2015). Natural variability of systems may depend on such uncertain factors as weather conditions, population growth or macroeconomic indicators. It is possible to quantify natural variability via uncertainty analyses; however, doing so requires careful consideration of the historical data because a probability distribution must be generated that represents the parameters of interest (Loucks and van Beek 2017).

2.2. Epistemic uncertainty

This type of uncertainty is caused by limited knowledge of the system. In contrast to aleatory uncertainty, epistemic uncertainty can be reduced through additional research (Ascough et al. 2008). However, according to van der Keur et al. (2008), additional research may also increase this type of uncertainty by revealing new aspects of the system not considered previously. Epistemic uncertainty may result from measurement error, systematic error during data collection and analysis, imperfect model representations of the system, and the researcher's subjective judgment (Walker et al. 2003).

Measurement error

This type of error occurs because a measurement almost always fails to represent the true value of the data point being measured (Walker et al. 2003). Regan et al. (2002) further differentiate measurement error into operator error (e.g., imperfections in observational techniques) and instrument error (e.g., imperfections in measuring equipment). Measurement errors can be easily estimated using statistical methods involving multiple samples. If such an error can be estimated, it can also be addressed in simulation models via stochastic techniques (Uusitalo et al. 2015).

Systematic error

A systematic error results from bias in the sampling procedure or measurement equipment (Regan et al. 2002). Unlike measurement error, it does not vary around the true value; therefore, it cannot be estimated. This type of error is extremely difficult to detect. Furthermore, if it goes unnoticed, it can have cumulative effects on the model results (Uusitalo et al. 2015). The only way to deal with systematic error is to find it in advance and eliminate it.

Model uncertainty

Simulation models are always imperfect representations of real systems; therefore, there is always some degree of uncertainty associated with them. Model uncertainty can, for example, arise from the choice of variables or parameters to be included in the model or from the choice of functional forms used in the model. This type of uncertainty is difficult to quantify (Walker et al. 2003).

Subjective judgment

The uncertainty caused by subjective judgment results from the subjective interpretation of data (Uusitalo et al. 2015). It is more likely to arise when data are lacking, for example, for estimating model parameters, and expert judgment must be exercised (Regan et al. 2002).

2.3. Linguistic uncertainty

According to Regan et al. (2002), linguistic uncertainty can arise from vagueness in language, context dependence, ambiguity, the indeterminacy of theoretic terms, and underspecificity.

Vagueness

Vagueness results from the fact that our natural, as well as scientific, vocabulary has gaps that permit cases in which exact descriptions of some quantities or entities are unavailable (Ascough et al. 2008). In other words, there are borderline cases that do not fit into specific categories (Regan et al. 2002).

Context dependence

Such uncertainties arise from the failure to specify the context in which a statement is made. This type of uncertainty can be avoided with an exact specification of the context.

Ambiguity

This type of uncertainty occurs because words often have multiple meanings. It arises when it is unclear as to which meaning is intended (Ascough et al. 2008). Problems with ambiguity often come about when data are collected from multiple sources.

Indeterminacy of theoretical terms

Uncertainty stemming from this source results from future usages of theoretical terms not being constrained by past usage (Regan et al. 2002). The indeterminacy of theoretical terms can make such terms ambiguous.

Underspecificity

Underspecificity results from the unwanted generality in data or statements (Ascough et al. 2008). For example, the statement that climate change will increase the probability of extreme weather events is underspecified because it leaves us wondering: In which period of time will this increase occur? What does the word "increase" imply? In which regional context is the statement true?

In this thesis, the term "uncertainty" refers to aleatory uncertainty because we consider the uncertainty resulting from crop yields variability which to a large extent is caused by natural variability of weather conditions.

CHAPTER 3

Multiple rotations of Gaussian quadratures: an efficient method for uncertainty analyses in large-scale simulation models

Chapter 3

3. Multiple rotations of Gaussian quadratures: an efficient method for uncertainty analyses in large-scale simulation models[1]

3.1. Abstract

Concerns regarding the impact of climate change, food price volatility, and weather uncertainty have motivated users of simulation models to consider uncertainty in their simulations. One way of doing so is to integrate uncertainty components in the model equations, thus turning the model into a problem of numerical integration. Most of these problems do not have analytical solutions, and researchers, therefore, apply numerical approximation methods. This chapter presents a novel approach to conducting an uncertainty analysis as an alternative to the computationally burdensome Monte Carlo-based (MC) methods. The developed method is based on the degree 3 Gaussian quadrature (GQ) formulae, and is tested using three large-scale simulation models. While a standard single GQ method often produces low-quality approximations, the results of this study demonstrate that the proposed approach reduces the approximation errors by a factor of 9 using only 3.4% of the computational effort required by the MC-based methods in the most computationally demanding model.

[1] This chapter is based on and to a large extent identical with Stepanyan et al. (2021) and the predecessors of that article (Stepanyan et al., 2019b; Stepanyan, 2018a; Stepanyan et al., 2018b).

3.2. Introduction

3.2.1. Uncertainty in simulation modeling

Simulation models are an established tool for assessing the impact of an exogenous shock, such as political or biophysical changes in ecological, economic, and social systems. Such models are also widely applied in analyses of agro-environmental systems and land-use changes. However, because all models are imperfect representations of real-world systems and accurate input data are not always available, the robustness of the model results needs to be addressed. In the context of uncertainty analysis (UA), Sheikholeslami et al. (2019) defined robustness as the stability of the results, *i.e.*, lower variability of the results obtained by solving a model with a sample of parameter values drawn from a probability distribution indicates a higher degree of robustness. Interested readers are directed to Kwakkel et al. (2016) for a comparison of different robustness metrics.

In addition, the uncertainty of the model results, owing to the real-world volatility of variables such as the weather, has been a frequent subject of analysis. A standard approach to tackling uncertainty in simulation models depicting agro-environmental systems is to incorporate uncertain terms[2] sampled from a probability distribution. This allows us to address not only issues of robustness but also a wide range of policy questions related to uncertainty. Simulation model analyses that use such terms to depict uncertainty can be classified into two main groups according to their purpose. The first group applies a systematic sensitivity analysis (SSA) regarding uncertain model parameters, typically referred to as epistemic uncertainty resulting from a lack

[2] Some studies refer to such uncertain terms as stochastic; see Beckman et al. (2011), Gouel and Jean (2013), and Pianosi et al. (2016). We also follow this convention in this thesis.

of knowledge (Uusitalo et al. 2015) (e.g., Arndt and Hertel 1997; Valenzuela et al. 2007; Beckman et al. 2011; Villoria et al. 2013; Cho et al. 2016). The second group explicitly considers the uncertainties inherent in the input variables, such as the weather, by describing such variables with probability distributions and producing distributions of the model outputs under an input uncertainty (e.g., European Commission 2018; Lammoglia et al. 2018; OECD/FAO 2018). The latter group is a type of UA (Loucks and van Beek 2017). The uncertainty considered by the second group is known as aleatory uncertainty (Uusitalo et al. 2015). In simulating agro-environmental systems, many studies have addressed the policy implications of uncertainty (Westhoff et al. 2005; Hertel et al. 2010; Moss et al. 2010; Verma et al. 2011; Gouel and Jean 2013). In this article, the term "uncertainty" refers to aleatory uncertainty because we consider the uncertainty resulting from crop yield variability to be due to weather uncertainty.

3.2.2. Uncertainty analysis as a numerical integration problem

To quantify uncertainty in simulation models, researchers normally apply numerical approximation methods because, in most cases, such problems do not have analytical solutions (Arndt 1996). One approach to modeling uncertainty is to consider it as a problem of numerical integration. Consider the following simple example of UA in a simulation model: Let x be an exogenous variable or parameter, g(x) be the probability density function describing the uncertainty of x supported on a particular interval [a, b], and f(x) be a function in the model for which we wish to find the expected value:

$$E[f(x)] = \int_a^b f(x)g(x)dx. \tag{3.1}$$

In many applications, such integrals cannot be evaluated directly because they are not given in a closed form. Instead, numerical integration methods must be used. To this end, we choose *n* points x_k within the domain of integration, or so-called nodes, with associated weights w_k, and we approximate integral (3.1) using the following finite sum:

$$\tilde{E}[f(x)] = \sum_{k=1}^{n} f(x_k) w_k. \tag{3.2}$$

The nodes and their weights for such a quadrature formula are chosen in such a way that approximation (3.2) yields the same results as (3.1) for polynomials of low degree. Consequently, the degree of accuracy of quadrature formula (3.2) is defined as follows:

$$max\{M \in N_0 : E[x^m] = \tilde{E}[x_m] \; for \; m = 0,\ldots,M\}. \tag{3.3}$$

This approach approximates the continuous probability distribution with density function *g(x)* in (3.1) based on a finite discrete probability distribution. Thus, the finite discrete probability distribution is chosen to maximize the number of shared moments (e.g., expected value, variance, skewness, or kurtosis) with a continuous probability distribution.

This approach can also be used for multivariate integrals; in this case, we refer to approximations of type (3.2) as a cubature formula. As an example, consider the case of a multivariate normal distribution with mean vector $\vec{\mu}$ and covariance matrix Σ. Then, $g(\vec{x})$ is given by the following:

$$g(\vec{x}) = \frac{1}{\sqrt{(2\pi)^d \, det(\Sigma)}} exp(-\frac{1}{2}(\vec{x}-\vec{\mu})^T \Sigma^{-1}(\vec{x}-\vec{\mu})). \tag{3.4}$$

Note, however, that this implies that the domain of integration is no longer bounded, but instead is all R^n (Euclidean space). There is a wide range of methods for choosing the nodes and their weights. Those most frequently used are discussed below.

3.2.3. Sampling and analysis methods

Methods for SSA or UA can be categorized as local or global. Local methods consider the uncertainty of the model output against variations of a single input factor (Pianosi et al. 2016). The disadvantage of this approach is that it does not consider interactions among input factors and therefore only provides a limited view of model uncertainty (Douglas-Smith et al. 2020). By contrast, global methods evaluate the input uncertainty over the entire range of input space, varying all input factors simultaneously (Matott et al. 2009). This type of method allows for a more comprehensive depiction of model uncertainty by accounting for the interactions among the input factors (Saltelli and Annoni 2010). Saltelli et al. (2019) claim that SSA/UA should always be based on global methods because local methods do not adequately represent models with nonlinearities. However, considering the computational capacity required to produce statistically robust results, conventional methods of global SSA/UA suffer from poor computational efficiency (Razavi and Gupta 2016a), which is one of the factors explaining the limited use of these methods compared to local methods (Douglas-Smith et al. 2020).

Douglas-Smith et al. (2020) analyzed 11,625 studies applying or introducing SSA/UA techniques within the field of environmental science from 2000 to 2017. The study shows that, during the time period investigated, there was a sharp increase (by a factor of 5) in the number of publications that apply such techniques, whereas the trend of

studies introducing and applying novel tools for SSA/UA has remained largely flat. Despite the fact that SSA/UA is becoming more relevant, researchers still mainly apply conventional methods, which are computationally burdensome.

The remainder of this section discusses some of the most established and widely applied SSA/UA methods, presenting their advantages and drawbacks.

The Monte Carlo (MC) method was introduced by Metropolis and Ulam (1949) and has been one of the most commonly used sampling techniques. The basic idea behind the MC method is to perceive integration as a probabilistic problem and approximate its solution using statistical experiments. Thus, the underlying logic is to choose the nodes randomly. According to the law of large numbers, the numerical result will then be close to the correct value if the number of points is sufficiently large. Although this method is easy to apply and is extremely effective, it is inefficient because it requires large sample sizes. According to Haber (1970), the MC sample size should range from 40,000 to 100,000 to obtain an error below 1%. The main disadvantages of this method are therefore slow convergence rates with increasing sample sizes (Engels 1980) and high computational requirements. Because a large number of iterations is necessary for obtaining reliable results (Artavia et al. 2015; Razavi and Gupta 2016a), its application in large-scale simulation models is extremely demanding, if not infeasible, in terms of the computational requirements, time, and data management costs (e.g., European Commission (2018)).

To achieve a higher convergence rate using MC-based methods, a type of stratified sampling is typically applied (Saltelli et al. 2008). The idea behind this approach is to divide the parameter space into sub-regions (strata) and assign an equal quota of samples to each sub-region (Norton 2015). In this case, the sub-regions do not

necessarily need to be equally weighted. Hence, the sample size will be equal to $N \cdot S$, where *N* is the number of strata, and *S* is the number of points selected from each stratum. This strategy has several advantages over pure random sampling. First, it ensures that the randomly selected points are spread somewhat evenly across the domain of the distribution according to the probability mass, thus increasing the rate of convergence considerably. Consequently, the sample size required to obtain results of equal quality is much smaller than that used in random sampling. The challenge with this method is the definition of the strata and the calculation of their probabilities (Saltelli et al. 2008).

The Latin hypercube sampling (LHS) technique is a compromise between utilizing pure random sampling and stratified sampling. It divides the domain of the probability distribution into *N* subsets of equal probability, where *N* is the sample size, and then randomly selects one point from each subset (Helton and Davis 2003). In contrast to stratified sampling, there is no need to define the strata or calculate their probabilities. This method ensures full coverage of the entire parameter space (Norton 2015).

As the main advantage of all MC-based methods, the accuracy of the approximation is independent of the degree of smoothness of the integration function. In addition, such methods are effective in revealing non-linearities. Nonetheless, they require thousands of iterations for each input factor and can be extremely demanding computationally, particularly for large-scale simulation models that are computationally intensive (Razavi and Gupta 2016a).

Because no predetermined sample size fits all models, often—and typically driven by the computational feasibility—SSA/UA are applied in large-scale simulation models using *ad hoc* and relatively small sample sizes that may limit the quality of the

approximations (Valin et al. 2015; OECD/FAO 2017; Villoria and Preckel 2017; Mary et al. 2018)[3]. This was also recognized by Sarrazin et al. (2016), who stated that in environmental applications with frequently complex models and computationally demanding simulations, a tradeoff exists between the robustness of the results and the computational costs[4]. Nevertheless, other studies have suggested various approaches to convergence evaluations. For example, Pianosi et al. (2016) suggest evaluating the convergence using sub-samples from the original sample and comparing the sensitivity indices of the results obtained from the sub-samples with the results obtained from the original sample. Yang (2011) suggests gradually increasing the sample size and observing the behavior of the coefficient of variation of the results.

Variance-based methods are designed to evaluate the impact of the variability of the input parameters on the overall variability of the output (Norton 2015). Some of the more well-known methods falling under this category are the Fourier amplitude sensitivity test (FAST) and the Sobol' method (Douglas-Smith et al. 2020). Because these methods are based on the MC algorithm, they become computationally demanding as the number of considered input factors increases (Pianosi et al. 2016). For example, the Sobol' method requires $N \cdot (2n + 2)$ points, where N is the chosen MC sample and n is the number of input factors (Yang 2011). As an advantage of these methods, however, the properties of the model they are applied to do not influence the quality of the results (Saltelli et al. 2008).

Derivative-based methods can be viewed as extensions of local UA methods. The basic idea behind these methods is to compute the partial derivatives of the model output

[3] These studies applied 550, 190, 300, and 10,000 points, respectively.
[4] However, it should be acknowledged that there are also studies that apply formal convergence evaluation criteria when conducting an uncertainty/sensitivity analysis, see Saltelli et al. (2010), Pianosi et al. (2016), and Razavi and Gupta (2016b).

concerning each model input. Thus, these values can be interpreted as local sensitivity indices to rank the input factors according to their influence on the model output (Razavi et al. 2019). As the main disadvantage of these methods, the derivatives are only computed at the base points of the model inputs and do not provide information regarding the rest of the input space (Saltelli et al. 2008). The Morris method, also known as the elementary effects (EE) method, is a derivative-based approach (Morris 1991) that computes the partial derivatives of the model outputs with respect to a sample of randomly selected model inputs. Each sample's mean and standard deviation is then considered as an uncertainty measure. For example, a higher mean value indicates the importance of the factor for the output, and a higher standard deviation indicates the non-linearity of the factor to the output and a strong interaction with other factors (Norton 2015). The EE method requires $N \cdot (n+1)$ model evaluations, where N is the MC sample size and n is the number of factors (Saltelli et al. 2008). This method has two main drawbacks. First, it is impossible to quantify the contribution of each factor to the output variability. Second, it is impossible to distinguish the factor non-linearity from interactions with other factors (Yang 2011).

Two strategies can be applied when a UA is too computationally demanding. First, an emulator can be used as a low-degree substitute, and second, the efficiency of the computationally demanding method can be improved (Song et al. 2012).

According to O'Hagan (2006), an emulator is a statistical approximation of the original simulation model. If this approximation is sufficiently precise, it can substitute for the original simulation model in applying a costly SSA/UA. For example, Zhan et al. (2013) proposed a global SA analysis method that combines the Morris method with a statistical emulator to reduce the computational costs. Although other methods also

exist, emulators are mostly based on Gaussian processes and represent a probability distribution for a desired function (O'Hagan 2012; Uusitalo et al. 2015). An emulator is based on a large sample of results from previously conducted simulations (O'Hagan 2012). According to Stanfill et al. (2015), emulator-based methods can accurately estimate the first-order sensitivity indices using half the number of computer model evaluations compared to traditional MC-based methods. As a disadvantage of using an emulator, it introduces numerical challenges related to model calibration and validation (Pianosi et al. 2016).

Gaussian quadratures (GQs) are a family of methods designed for efficiently and accurately approximating definite integrals (Arndt et al. 2015). Being a static estimator, GQ requires a minimal number of iterations ($2n$, where n is the number of uncertain input factors) to reproduce the second central moments of a joint probability distribution (Haber 1970). According to Schürer (2003), the methods based on GQ are expected to be the most efficient for low-degree polynomials, *i.e.*, for smooth integrands. This method is discussed more thoroughly in Section 3.3.

Other sampling approaches have also been designed for specific SSA/UA methods and are based on a simple random sampling, for example, sampling approaches for the FAST method (Cukier et al. 1973) and for calculating the Sobol' sensitivity indices (Saltelli 2002). Interested readers are directed to a review by Gan et al. (2014).

As an important conclusion from this discussion on SSA/UA methods, there is always a compromise between the computational requirements and the output reliability when choosing the method. The choice of method does not depend solely on the dimensionality of the problem, but also on the smoothness of the integrand, *i.e.*, the number of times the function is continuously differentiable (Arndt and Preckel 2006).

GQ methods outperform MC-based methods in terms of efficiency and accuracy for smooth integrands. For highly nonlinear integrands, by contrast, MC-based methods may be more suitable because they are neither dependent on the smoothness of the integrand nor on the dimensionality of the problem (Schürer 2001, 2003).

After the initial uptake when applying the GQ methods in large-scale simulation models (Arndt and Hertel 1997; Valenzuela et al. 2007; Villoria et al. 2013), Artavia et al. (2015) found that, depending on the initial position of the octahedron from which the rotation starts, the quality of the approximation differs. In addition, a recent study by Villoria and Preckel (2017) pointed out inaccuracies in results based on GQ methods applied in the global trade analysis project (GTAP) model. Specifically, large differences have been found in the first three moments of the probability distributions of the results produced by GQ and MC. To address these inaccuracies, this chapter presents a novel approach to the reduction of the approximation error for GQ methods, named multiple rotations of Gaussian quadratures (MRGQ). The MRGQ method aims at improving the quality of the approximations using traditional GQ methods while keeping the computational requirements low. It is primarily designed for computationally demanding models, where the cost of applying MC-based methods without consideration of the emulators is prohibitively high[5].

The remainder of this chapter is organized as follows: Section 3.3 provides a short overview of the theoretical background of Stroud's order 3 Gaussian quadratures.

[5] The cost or efficiency of a method is usually assessed by the number of iterations required to obtain statistically robust results (Razavi and Gupta 2016a). This is particularly relevant for computationally demanding simulation models. This is the case for example, for models with global coverage, such as the CAPRI model (Britz and Witzke 2014) and the EPIC-IIASA model (Balkovič et al. 2014), recursive-dynamic models such as the Aglink-Cosimo model (OECD/FAO 2015) or gridded models such as GLOBIOM (Havlík et al. 2011; Havlík et al. 2014), which can produce results on a 10 km × 10 km grid-level. These models comprise hundreds of thousands of variables and equations and hence require a large computational capacity for multiple solutions.

Section 3.4 introduces the proposed MRGQ method along with an example. It also details the approach used to generate a benchmark for evaluating the quality of the approximations made using GQ and the proposed MRGQ method. Section 3.5 provides an overview of the simulation models applied to compare the results between the MRGQ and GQ methods. In Section 3.6, the approximation results generated by GQ and MRGQ are evaluated by comparing them against an LHS-benchmark. Sections 3.7 and 3.8 offer a discussion and some concluding remarks with respect to the potential of the MRGQ method.

3.3. Theoretical background: Stroud's Gaussian quadratures

The method presented in this section refers to the degree 3 quadrature formulae by Stroud (1957), aiming to obtain results with a certain degree of accuracy using the least possible number of points. Stroud's (1957, p. 259) theorem states the following:
As a necessary and sufficient condition in which 2n points $v_1,\ldots, v_n$ and $-v_1,\ldots, -v_n$ form an equally weighted numerical integration formula of degree 3 for a symmetrical region R, these points form the vertices of a Q_n whose centroid coincides with the centroid of the region and lie on an n-sphere of radius $r = \sqrt{nI_2/I_0}$.

Here, Q_n is a regular, n-dimensional generalized octahedron being integrated into an n-sphere, I_0 is the volume of R, and I_2 is the integral of the square of any variables over region R. Region R is symmetric in the sense of Stroud's theorem if it is invariant under the group of automorphisms of an n-cube (Stroud 1957, p. 257). Figure 3.1 depicts a graphical representation of the theorem, which indicates that, to obtain an n-dimensional Gaussian quadrature formula of degree 3 for an n-dimensional cube, we must use 2n points, which are the vertices of a regular n-octagon (points 1–6 in Figure 3.1), the centroid of which is the centroid of the cube. Because we have 2n quadrature

points, which are supposed to be equally weighted, each weight must equal 1/2n. If these conditions are met, an approximation with an accuracy of degree 3 can be obtained.

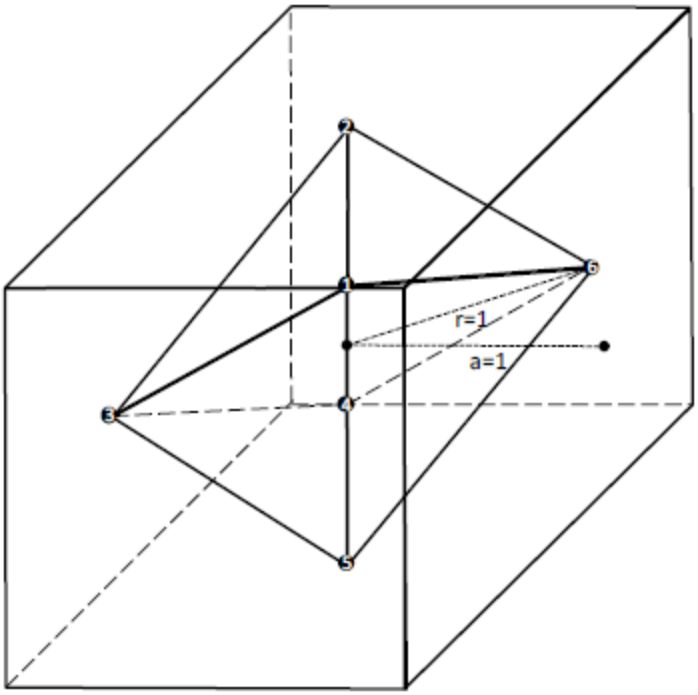

Figure 3.1. Graphical representation of Stroud's theorem for degree 3 quadrature formulae.

Notation: a, half of the side length of the cube; r, the radius of the n-octahedron.
Source: Artavia et al. (2015)

Stroud, however, encountered a problem in that whenever the dimensionality is greater than 3, the vertices fall outside of the integration region, yielding unusable formulae. This problem can be observed in the calculation below, which is adopted from Artavia et al. (2015).

The volume of an n-cube (C^n) with vertices (±a, ±a,…, ±a) can be obtained as follows:

$$I_0 = \int_{C^n} x_i^0 d\vec{x} = (2a)^n. \tag{3.5}$$

The integral of the square of any variable over this region is

$$I_2 = \int_{C^n} x_i^2 d\vec{x} = \int_{C^{n-1}} d\tilde{\vec{x}} \int_{[-a,+a]} x_i^2 dx_i = (2a)^{n-1} \left[\frac{1}{3} x_i^3 \right]_{-a}^{+a} = (2a)^{n-1} \frac{2}{3} a^3 = \frac{2^n}{3} a^{n+2}. \quad (3.6)$$

Here, $\tilde{\vec{x}} \in R^{n-1}$is the vector $\vec{x}$ with the coordinate x_i omitted. This yields the radius of the octahedron:

$$r = \sqrt{n \frac{I_2}{I_0}} = \sqrt{n \left(\frac{2^n}{3} a^{n+2} / 2^n a^n \right)} = \sqrt{n \frac{a^2}{3}} = a \sqrt{\frac{n}{3}}. \quad (3.7)$$

In the case considered in Figure 3.1, we deal with a three-dimensional cube with vertices (±1, ±1, ±1), and for n = 3, we obtain r = 1. However, note that for n > 3, we have r > a, and thus the vertices of the n-octahedron lie outside the n-cube.

As a solution to this problem, Stroud (1957) suggested the following formula to rotate the octahedron and bring the quadrature points back into the integration region. For k = 1,…, 2n, let Γ_k denote the quadrature point $(\gamma_{k,1}, \gamma_{k,2}, \ldots, \gamma_{k,n})$, where

$$\gamma_{k,2j-1} = \sqrt{\frac{2}{3}} \cos\left(\frac{(2j-1)k\pi}{n} \right), \quad (3.8)$$

$$\gamma_{k,2j} = \sqrt{\frac{2}{3}} \sin\left(\frac{(2j-1)k\pi}{n} \right), \quad (3.9)$$

for $j = 1, \ldots, [n/2]$, where $[n/2]$ is the greatest integer not exceeding n/2. In addition, if n is odd,

$$\gamma_{k,n} = \frac{(-1)^k}{\sqrt{3}}. \quad (3.10)$$

The quadrature points generated by these formulae fulfill the three prerequisites mentioned above.

Arndt (1996) adapted Stroud's formulae for integrals over all R^n (Euclidean space) with the multivariate standard normal distribution as a weight function. Arndt's formulae are simply the Stroud points multiplied by $\sqrt{3}$, which is derived from the fact that the value of the radius $\left(r = \sqrt{n\frac{I_2}{I_0}}\right)$ changes as follows:

$$I_0 = \int_{R^n} x_i^0 \frac{1}{(2\pi)^{n/2}} e^{-\frac{\|\vec{x}\|^2}{2}} d\vec{x} = (1)^n = 1, \tag{3.11}$$

$$I_2 = \int_{R^n} x_i^2 \frac{1}{(2\pi)^{n/2}} e^{-\frac{\|\vec{x}\|^2}{2}} d\vec{x} = \int_{R^{n-1}} \frac{1}{(2\pi)^{(n-1)/2}} e^{-\frac{\|\tilde{\vec{x}}\|^2}{2}} d\tilde{\vec{x}} \int_R x_i^2 \frac{1}{(2\pi)^{1/2}} e^{-\frac{x_i^2}{2}} dx_i = (1)^{n-1} 1 = 1. \tag{3.12}$$

Here, $\|\vec{x}\|$ denotes the Euclidean norm of the vector $\vec{x} \in R^n$, and $\tilde{\vec{x}} \in R^{n-1}$ is the vector $\vec{x}$ with the coordinate x_i omitted; therefore, in particular, $\|\vec{x}\|^2 = \left\|\tilde{\vec{x}}\right\|^2 + x_i^2$.

It follows that

$$r = \sqrt{n\frac{I_2}{I_0}} = \sqrt{n}. \tag{3.13}$$

Therefore, Equations (3.8)–(3.10) must be adapted accordingly, and for the k^{th} quadrature point $\Gamma_k = \left(\gamma_{k,1}, \gamma_{k,2}, \ldots, \gamma_{k,n}\right)$, where k = 1, 2,…, 2n, we obtain the following:

$$\gamma_{k,2j-1} = \sqrt{2}\cos\left(\frac{(2j-1)k\pi}{n}\right), \tag{3.14}$$

$$\gamma_{k,2j} = \sqrt{2}\sin\left(\frac{(2j-1)k\pi}{n}\right), \tag{3.15}$$

for $j = 1, \ldots, [n/2]$, where [n/2] is the greatest integer not exceeding n/2, and if n is odd,

$$\gamma_{k,n} = (-1)^k. \tag{3.16}$$

The GQ points generated by Stroud's (1957) formulae, that is, (3.8)–(3.10), have a restricted variation around a mean of no more than $\sqrt{2/3}\sigma_i$ on each coordinate axis. Consequently, the variation of the GQ points proposed by Arndt (1996) is restricted to no more than $\sqrt{2}\sigma_i$ on each coordinate axis, where σ_i is the standard deviation of the *i*-th uncertain input factor. This sampling interval, however, can be broadened by a desired factor using the method proposed by Preckel et al. (2011). To endow the finite distribution with the desired covariance matrix Σ, the sampling points need to be multiplied by a square matrix A satisfying $\Sigma = AA^T$. There are several standard methods that can be used to obtain A from Σ, such as eigenvalue decomposition, Cholesky factorization, or reverse Cholesky factorization (Artavia et al. 2015). Therefore, the matrix of the final quadrature points can be obtained as $GQ = A\Gamma + \vec{\mu}[1 \quad \ldots \quad 1]$, where $\vec{\mu}$ is the vector of the mean values (e.g., the base values of the input factors). In this study, we use the eigenvalue decomposition technique.

3.4. Methods

3.4.1. Benchmark generation

In the first step, we generate a reliable benchmark against which the results obtained by the proposed MRGQ method are compared. We use the well-established LHS technique and systematically determine a sufficient sample size for each model. To this end, we solve each model using the LHS technique with a converged sample size, that is, by following the convergence evaluation method suggested by Yang (2011), we solve the model with a small sample size and gradually increase it[6]. We observe the behavior of the coefficients of variation (CVs) of two variables: the total production of each crop for which the productivity was shocked and the respective price levels. These two variables are the most relevant for simulated shocks that depict model uncertainty. In general, the variables most relevant to the respective study should be selected. The stop criterion is satisfied when the percentage of change in the results of interest, compared to the results from the previous sample size, stays within an interval of [-1%, 1%]. The advantages of using the CVs as an indicator are twofold: first, this measurement is dimensionless, thus facilitating a comparison, and second, it captures both the first and second moments of the data.

[6] For all models, we used sample sizes of 1,000 and 2,000 as well as further increases in sample sizes in increments of 2,000. Depending on the complexity of the model, we used sample sizes smaller than 1,000 as *ad hoc* choices.

3.4.2. MRGQ method

Artavia et al. (2015) showed that the quality of the GQ results depends strongly on the selected rotation of Stroud's octahedron. To counteract this effect, we use several families of GQ points generated from different random rotations of Stroud's octahedron. To this end, we randomly choose k of n! possible permutations in the n coordinates. Owing to the structure of Stroud's matrix, the easiest way to introduce random rotations is by randomly permuting the rows of Stroud's matrix. This is achieved by multiplying the matrix from the left by a permutation matrix, that is, a matrix containing a single 1 in each row and column and zeros everywhere else. Using k permutations increases the number of quadrature points by a factor of k, and at the same time, considerably improves the quality of the output, as will be shown in the results section.

Following the insights of Artavia et al. (2015), we investigate how the initial position of Stroud's octahedron from where we started the rotation affects the final results of the GQ approximation. We generated ten series of quadratures through ten random rotations of the octahedron for the GLOBIOM model, and 20 series from 20 random rotations for each of the other 2 models. Note that each series contains only 2n points, where n is the number of uncertain variables. The number of random rotations is selected arbitrarily, considering the available computational capacities. After solving the models with the quadrature points generated by each individual rotation, we also solve them using the MRGQ method.

To evaluate the quality of the results of the MRGQ method, we compared them to the previously generated LHS benchmark. In the case of the dynamic CGE, we follow the approach of Arndt and Thurlow (2015) and observe only the final 5-year average of the

results, assuming that doing so will allow us to capture the cumulative effects of the uncertain input factors from previous time periods. The MRGQ method is implemented in four steps:

3.4.2.1. Step 1: Calculating the Stroud matrix

The first step is to generate a Stroud matrix for the joint standard normal distribution using Equations (3.14)–(3.16). For example, in the case of a three-dimensional problem, the Stroud matrix will have the following form:

$$\Gamma = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\sqrt{2} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \sqrt{2} \\ \sqrt{\frac{3}{2}} & \sqrt{\frac{3}{2}} & 0 & -\sqrt{\frac{3}{2}} & -\sqrt{\frac{3}{2}} & 0 \\ -1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix}.$$

3.4.2.2. Step 2: Transforming the covariance matrix

To incorporate the desired covariance structure and the base values into the Stroud matrix, the first step is to derive a covariance matrix of the uncertain input factors. For example, in this study, the covariance matrix is derived from historical data using the methodologies of Burrell and Nii-Naate (2013) and Araujo-Enciso et al. (2017). As an example, let us consider the following covariance matrix Σ and the vector $\vec{\mu}$ of the base values, which in this case are randomly generated for demonstration only:

$$\Sigma = \begin{bmatrix} 0.289558 & 0.246504 & -0.583676 \\ 0.246504 & 1.430970 & 0.215241 \\ -0.583676 & 0.215241 & 1.699880 \end{bmatrix}, \ \vec{\mu} = \begin{bmatrix} 1.46798 \\ 7.88187 \\ 5.59115 \end{bmatrix}.$$

As described in Section 3.3, to endow a finite distribution with the desired covariance matrix Σ, we need to multiply Stroud's matrix, generated in Step 1, by a square matrix A satisfying $\Sigma = AA^T$. To obtain the square matrix A, we apply the diagonalization method according to the following:

$$\Sigma = UDU^T = (U\sqrt{D})(\sqrt{D}U^T) = AA^T, \tag{3.17}$$

where U is the matrix of the eigenvectors of Σ, and D is the diagonal matrix of the eigenvalues of Σ. From the example above, we obtain the following:

$$D = \begin{bmatrix} 1.94088 & 0 & 0 \\ 0 & 1.46611 & 0 \\ 0 & 0 & 0.0134251 \end{bmatrix},$$

$$U = \begin{bmatrix} -0.289240 & 0.281216 & 0.915018 \\ 0.250202 & 0.944856 & -0.211297 \\ 0.923980 & -0.167823 & 0.343651 \end{bmatrix}.$$

Solving Equation (3. 17) yields the following:

$$A = U\sqrt{D} = \begin{bmatrix} -0.289240 & 0.281216 & 0.915018 \\ 0.250202 & 0.944856 & -0.211297 \\ 0.923980 & -0.167823 & 0.343651 \end{bmatrix} \times \begin{bmatrix} 1.39315 & 0 & 0 \\ 0 & 1.21083 & 0 \\ 0 & 0 & 0.115867 \end{bmatrix} \tag{3.18}$$
$$= \begin{bmatrix} -0.402957 & 0.340505 & 0.106020 \\ 0.348570 & 1.144060 & -0.024482 \\ 1.287250 & -0.203205 & 0.039818 \end{bmatrix}.$$

3.4.2.3. Step 3: Incorporating the covariance structure into the Stroud matrix

The GQ points can now be generated using the equation below:

$$GQ = A\Gamma + \vec{\mu}[1...1] \tag{3.19}$$

$$= \begin{bmatrix} -0.402957 & 0.340505 & 0.10602 \\ 0.34857 & 1.14406 & -0.0244823 \\ 1.28725 & -0.203205 & 0.0398178 \end{bmatrix} \times \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\sqrt{2} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \sqrt{2} \\ \sqrt{\frac{3}{2}} & \sqrt{\frac{3}{2}} & 0 & -\sqrt{\frac{3}{2}} & -\sqrt{\frac{3}{2}} & 0 \\ -1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix} +$$

$$\begin{bmatrix} 1.46798 \\ 7.88187 \\ 5.59115 \end{bmatrix} \times [1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1]$$

$$= \begin{bmatrix} 1.49406 & 2.27597 & 1.93183 & 1.44191 & 0.659999 & 1.00414 \\ 9.55401 & 9.0121 & 7.4134 & 6.20973 & 6.75165 & 8.35034 \\ 6.21268 & 4.47188 & 3.73089 & 4.96962 & 6.71043 & 7.45141 \end{bmatrix}.$$

As can be seen from the final matrix obtained by Equation (3.19), the required sample size is equal to 2n, where n is the number of uncertain input factors.

3.4.2.4. Step 4: Generating the MRGQ points

To perform a random rotation of the GQ, we apply a randomly generated permutation matrix, e.g., $P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$. Thus, the randomly generated GQ_{Rand} matrix is calculated as follows:

$$GQ_{Rand} = AP\Gamma + \vec{\mu}[1...1] \tag{3.20}$$

$$= \begin{bmatrix} -0.402957 & 0.340505 & 0.106020 \\ 0.348570 & 1.144060 & -0.024482 \\ 1.287250 & -0.203205 & 0.039818 \end{bmatrix} \times \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\sqrt{2} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \sqrt{2} \\ \sqrt{\frac{3}{2}} & \sqrt{\frac{3}{2}} & 0 & -\sqrt{\frac{3}{2}} & -\sqrt{\frac{3}{2}} & 0 \\ -1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix}$$

$$+ \begin{bmatrix} 1.46798 \\ 7.88187 \\ 5.59115 \end{bmatrix} \times [1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1]$$

$$= \begin{bmatrix} 0.70893 & 1.24000 & 0.97754 & 2.22704 & 1.69597 & 1.95842 \\ 7.14741 & 9.47015 & 6.77244 & 8.61633 & 6.29359 & 8.99131 \\ 7.39906 & 6.93634 & 5.73805 & 3.78324 & 4.42460 & 5.44426 \end{bmatrix}.$$

This indicates that the application of the permutation matrix yields extremely different GQ points. Finally, to obtain the matrix of MRGQ points, we need to combine the GQ matrices generated by all different rotations:

$$MRGQ = \begin{bmatrix} 1.49406 & 2.27597 & 1.93183 & 1.44191 & 0.659999 & 1.00414 & 0.70893 & 1.24000 & 0.97754 & 2.22704 & 1.69597 & 1.95842 \\ 9.55401 & 9.0121 & 7.4134 & 6.20973 & 6.75165 & 8.35034 & 7.14741 & 9.47015 & 6.77244 & 8.61633 & 6.29359 & 8.99131 \\ 6.21268 & 4.47188 & 3.73089 & 4.96962 & 6.71043 & 7.45141 & 7.39906 & 6.93634 & 5.73805 & 3.78324 & 4.42460 & 5.44426 \end{bmatrix}.$$

Please note that working separately with both GQ families generated the above and taking the average yields the same result as taking the union of the two families and adjusting the weights accordingly. In this case, the weights are equal to $1/2 \cdot 1/6 = 1/12$.

3.5. Simulation models and data

The MRGQ approach is tested using three different simulation models covering environmental dimensions such as land-use and weather-driven yields, *i.e.*, a comparative-static, single-country computable general equilibrium (CGE) model based on the static applied general equilibrium model, ver. 2 (STAGE2) (McDonald and Thierfelder 2015), and extended for and applied to Bhutan (Feuerbacher et al. 2018) (called static CGE throughout this chapter); GLOBIOM (Havlík et al. 2011; Havlík et al. 2014), a global partial equilibrium (PE) model of the agricultural and forestry sectors; and a multi-sector recursive-dynamic CGE model for the Sudan (Diao and Thurlow 2012) (called dynamic CGE throughout this chapter). All models are programmed using the General Algebraic Modeling System.

In all models, we simulate the uncertainty of the crop yields resulting from weather and other environmental factors (such as the prevalence of disease), which constitutes a major determinant of agricultural price volatility. For this purpose, we use historical data from agricultural databases (FAOSTAT 2018; ICRISAT 2018) and national

institutions (MoAF 2016). Following Burrell and Nii-Naate (2013), we separate the uncertainty components from the historical crop yield data as deviations from the estimated trends for crops with sufficient data availability. Subsequently, uncertain input factors are generated. For example, let $y_{c,y}$ be the observed yield of crop c in year y, where $c = (1,2, ..., n)$ and $y = (1,2, ..., m)$, and $\hat{y}_{c,y}$ be the estimated trend for the same crop in the same year. Thus, the uncertainty component ($z_{c,y}$) is calculated as $z_{c,y} = y_{c,y} / \hat{y}_{c,y} - 1$. Following the same procedure for all variables, we generate the matrix of uncertainty components (deviates) $Z_{c \times y}$. The covariance matrix of the derived uncertainty components is used to generate the multivariate distributions from which the uncertain input factors are drawn, as explained in Section 3. Because the expected value of these input factors is equal to zero, it is irrelevant which crop yields are chosen as uncertain in this context.[7]

[7] In this chapter, the choice of uncertain yield variables is related to data quality and availability.

3.5.1. Static CGE

Static CGE is a single-country, comparative-static CGE model using the STAGE2 framework and has been documented extensively by McDonald and Thierfelder (2015). Static CGE extends the basic STAGE2 model to include a multi-level production structure of nested constant elasticity of substitution (CES) and Leontief fixed-coefficient technology functions. The demand system follows a two-stage linear expenditure system (LES)-CES nest, allowing for a substitution of commodities. The model extension and parameters are documented by Feuerbacher et al. (2018). The model is calibrated to a 2012 social accounting matrix for Bhutan (Feuerbacher et al. 2017) with multiple sectors, ten of which are crop-producing.

The model is run such that household saving rates are adjusted to meet a given level of investment. The exchange rate is flexible, and the foreign savings are fixed. Reflecting the short-term nature of the uncertain input factors, the model closures account for fixed land allocation (no land mobility across crop sectors), fixed government spending, and flexible government savings (all tax rates remain constant). The impact of the yield uncertainty is evaluated for all ten crop-producing sectors, namely, paddy, maize, wheat, pulses, vegetables, potatoes, spices, apples, citrus fruits, and other fruits and nuts. The uncertainty in the crop yields is modeled by shocking the respective crop sector's total factor productivity (TFP). The changes in TFP are expressed using the variable ADX_a for activity a in the following model equation depicting production:

$$QX_a = ADX_a \cdot (\delta_a^x \cdot QVA_a^{-rhoc_a^x} + (1-\delta_a^x) \cdot QINT_a^{-rhoc_a^x})^{\frac{-1}{rhoc_a^x}}, \tag{3.21}$$

where QX_a is the output of activity a, δ_a^x is the share parameter for the CES production function determining the aggregated amount of factors used, that is, aggregated value

added (QVA) and aggregated intermediates (QINT) used, and $rhoc_a^x$ is the substitution parameter. In addition, ADX_a is endogenously determined according to the following adjustment mechanism:

$$ADX_a = [(adxb_a + dabadx_a) \cdot ADXADJ] + (DADX \cdot adx01_a), \quad (3.22)$$

where adxb is the base value, dabadx is an absolute change in the base value, ADXADJ is a multiplicative adjustment factor, DADX is an additive adjustment factor, and adx01 is a vector consisting of zeros and non-zeros used to scale the additive adjustment factor. The uncertainty component ($rand_a$) is added to Equation (3.22) as follows:

$$ADX_a = (1 + rand_a) \cdot [[(adxb_a + dabadx_a) \cdot ADXADJ] + (DADX \cdot adx01_a)]. \quad (3.23)$$

3.5.2. GLOBIOM

GLOBIOM is a bottom-up, recursive-dynamic PE model with global coverage, integrating the agricultural, bioenergy, and forestry sectors (Havlík et al. 2011; Havlík et al. 2014). It is a linear programming model with a spatial equilibrium approach (Takayama and Judge 1971). The market equilibrium for agricultural and forestry products is computed based on a welfare-maximizing objective function subject to resource, technology, demand, and policy constraints. The model version applied in this study covers 31 regions globally and considers the 18 most important crops in terms of globally harvested quantities. Because this version of the model requires a large computational capacity, we use it in a comparative static framework, starting from a fixed 2010 solution and solving the model for only one time step (2020). We analyze the yield uncertainties of groundnuts, maize, rice, soybeans, and sugarcane grown in Indonesia, and of barley, groundnuts, sorghum, potatoes, dry beans, rice, wheat, sugarcane, maize, soybeans, cassava, and sweet potatoes grown in Brazil. In

GLOBIOM, at the national level, land-use data are based on FAOSTAT statistics, which are spatially allocated using data from the spatial production allocation model (SPAM) (You and Wood 2006). Production technologies, as indicated by SPAM data, are specified through Leontief production functions. Four different management systems (irrigated–high-input, rainfed–high-input, rainfed–low-input, and subsistence) are simulated using the biophysical process-based crop model EPIC (Williams 1995; Izaurralde et al. 2006) and fitted to the national averages of FAOSTAT yield data for approximately the year 2000 (average for 1998–2002). Over the course of a particular scenario, yields react through changes in the management system, spatial reallocations, or exogenous components representing technical change. For our analysis, uncertain yield shocks are applied as exogenous shifters in the same manner as shown in Equation (3.23) for all management systems.

3.5.3. Dynamic CGE

Dynamic CGE is an economy-wide, recursive-dynamic CGE model (Diao and Thurlow 2012) linked to the IMPACT modeling system (Robinson et al. 2015). The model is calibrated to the most recent social accounting matrix for the Sudan with multiple sectors, 26 of which are crop-producing (Siddig et al. 2018). The demand for the primary factors is governed by the CES functions, whereas the intermediate input demand is determined by the Leontief fixed-coefficient technology function. As in static CGE, we assume government savings to be flexible and all tax rates to be fixed. For the external balance, a flexible exchange rate is chosen, and the foreign savings are fixed. Finally, for the saving–investment identity, a fixed share of investment in terms of the absolute absorption is assumed, whereas household saving rates are endogenously adjusted in a uniform way to generate the necessary funds.

In the context of dynamic CGE, the uncertainty of the following crop yields was analyzed: irrigated cotton, irrigated and mechanized rain-fed sorghum, irrigated wheat, irrigated groundnuts, mechanized rain-fed millet, and mechanized and traditional rain-fed sesame. Similar to the static CGE, uncertainty components affect the TFP, as presented in Equation (3.23). Although the recursive-dynamic framework of the model is set up to project the period of 2018–2050, considering the huge computational requirements of the LHS approach, we conduct our study for the time interval of 2018–2025 to obtain a benchmark. As extreme weather shocks in Sudan occur in a cyclical manner (MEDP 2013), every five years on average, the uncertainty components are applied every fifth year, in this case, in 2018 and 2023.

3.6. Results

The benchmark results for each model and the results generated by the proposed MRGQ method are presented in the following two subsections.

3.6.1. Benchmark using the LHS method

The comparative-static single-country CGE model represents a model category that, unlike the other two models, is characterized by relatively low computational requirements. The convergence criterion in the production quantities is satisfied at 10,000 iterations. However, the convergence criterion in the prices is reached only at 20,000 iterations, which is subsequently selected as the benchmark sample size (Figure 3.2).

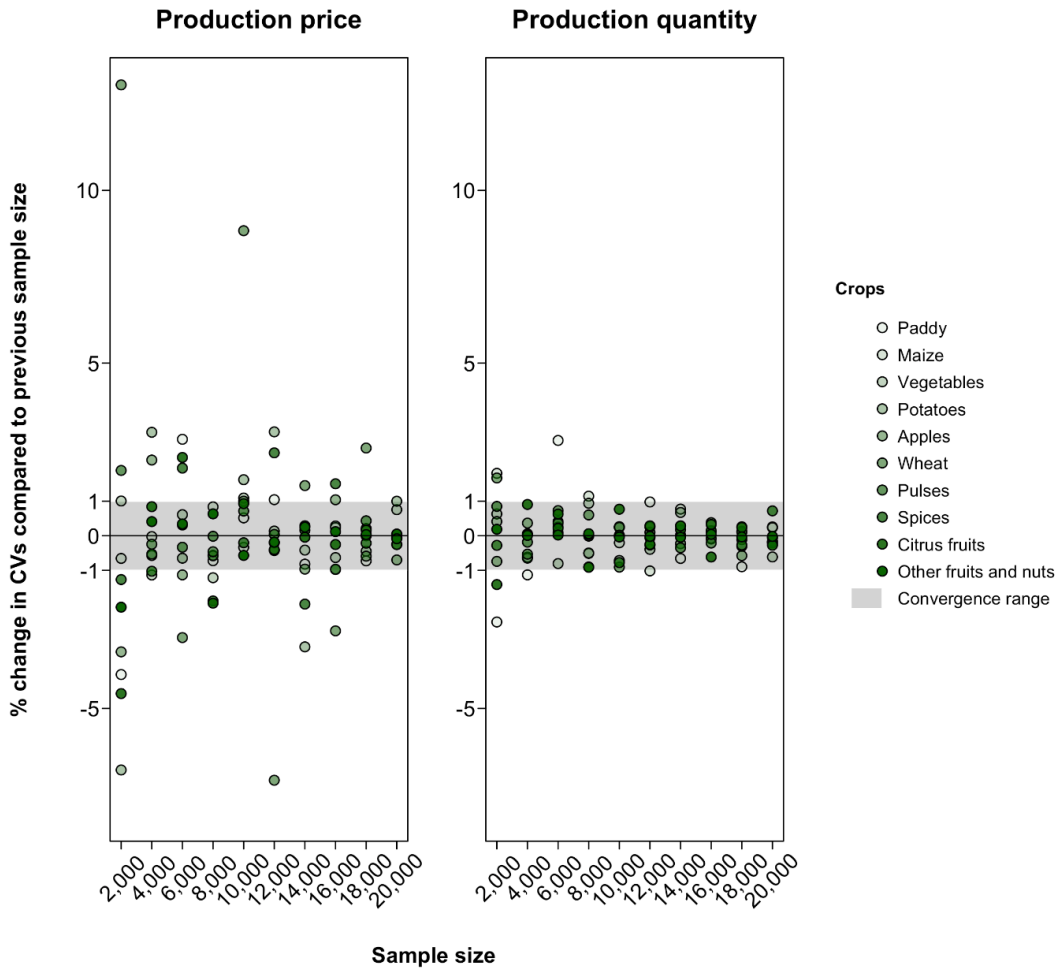

Figure 3.2. Convergence of the CVs of production prices and production quantities for static CGE.

The total factor productivity parameters of the respective crops are considered uncertain and are randomly drawn from a multivariate normal distribution using the LHS method. The starting sample size is 1,000. The sample size is gradually increased until the percentage of changes in the results compared with those obtained from the previous sample size remain within a ± 1% range.

For GLOBIOM, the number of iterations is increased to 10,000. At this point, however, the convergence criterion is not satisfied for all crops: 4 out of 17 price variables still exhibit changes slightly above the 1% threshold (1.46% at maximum). However, given the resources required to continue increasing the number of iterations (approximately 3,000 computer-hours for 12,000 iterations), we consider the results of 10,000 iterations as a reference because the limit of the available computational capacity was reached (Figure 3.3).

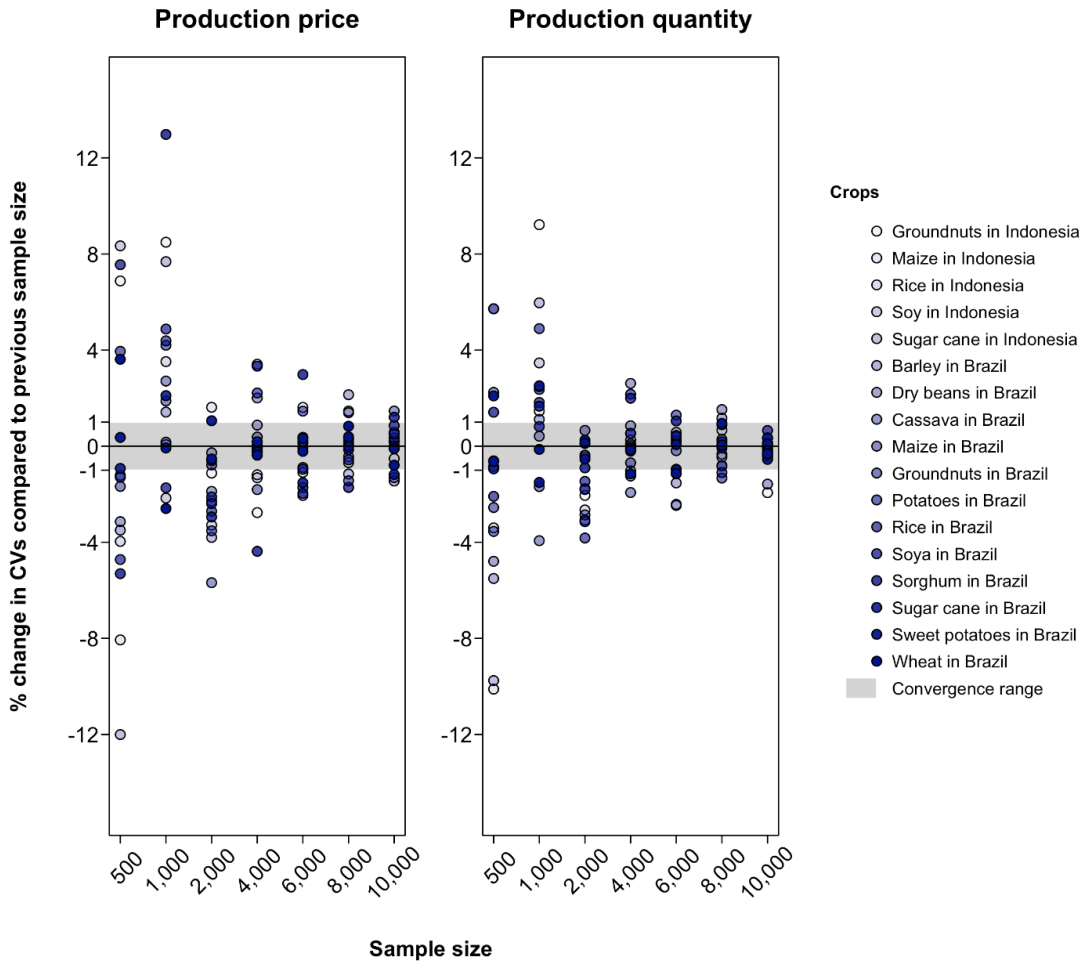

Figure 3.3. Convergence of the CVs of the production prices and production quantities for GLOBIOM.

The yields of the respective crops are considered uncertain and are randomly drawn from a multivariate normal distribution using the LHS method. The starting sample size is 100. The sample size is gradually increased until the percentage of changes in the results compared with those obtained from the previous sample size remain within a ±1% range.

For dynamic CGE, we evaluate the convergence by analyzing the behavior of the mean absolute CVs in the growth rates of the production and prices over the projected period. The convergence criterion for the price growth rate is reached at 12,000 iterations (Figure A.2). The convergence criterion for the production growth rate is reached at

14,000 iterations, which is chosen as the benchmark for the dynamic CGE model.

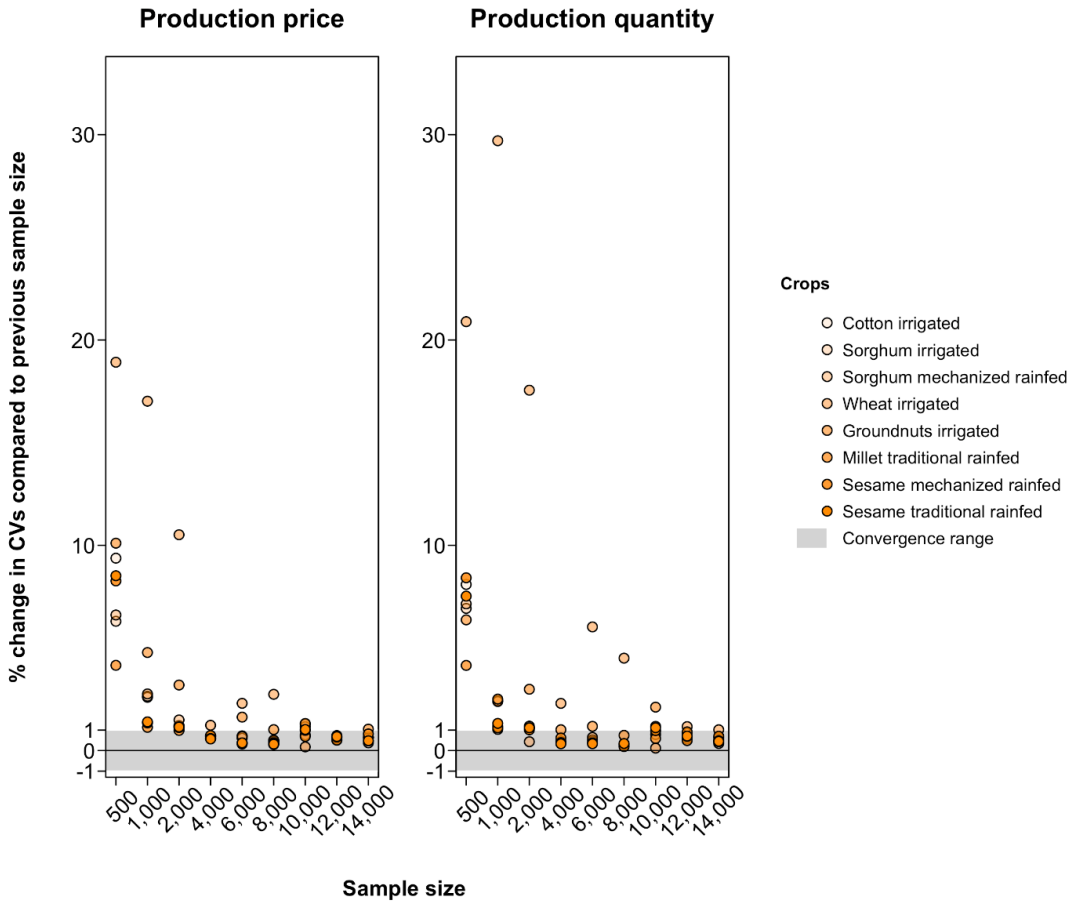

Figure 3.4. Convergence of the CVs of the average absolute production price and growth rates over the projected period for dynamic CGE.

The total factor productivity parameters of the respective crops are considered uncertain and are randomly drawn from a multivariate normal distribution using the LHS method. The starting sample size is 100 iterations. The sample size is gradually increased until the percentage of changes in the results compared with those obtained from the previous sample size remain within a ±1% range.

In the above-mentioned figures, one can also observe that the model dimensionality and complexity are positively correlated with the relevance of the increasing sample size required to reach the convergence of the CVs.

3.6.2. MRGQ results

Example results from each model are presented in Figures 3.5–3.7 as percent deviations from the benchmark results derived using the LHS method (for the complete results, see Figures 3.8–3.10). As the first observation, the bars demonstrate that, depending on the rotations of Stroud's octahedron, the generated quadrature points lead to different levels of quality compared to the benchmark results. The largest deviations in the CVs of the production and prices from the benchmark, presented in Figures 3.5 to 3.7, are −10% and +10%, +11% and −4%, and −14% and −16%, in the static CGE, GLOBIOM, and dynamic CGE models, respectively. Second, the dashed lines show that the proposed MRGQ method delivers results that are extremely close to the benchmark while also keeping the number of required iterations small compared to those required by the probabilistic methods. Table 3.1 shows the number of iterations used by the two methods for each model and the percentage of reduction in these numbers by the proposed MRGQ method as compared to the LHS. Together with the results presented in Figures 3.5, 3.6, and 3.7, this shows that the MRGQ method produces high-quality results using only a fraction of the iterations required by the LHS method, and thus substantially reduces the computational effort.

Table 3.1. Percentage of reduction in the iterations required by the MRGQ method compared to the converged sample size iterations required by the LHS method

	LHS	MRGQ	% reduction
Static CGE	20,000	400	98.0
GLOBIOM	10,000	340	96.6
Dynamic CGE	14,000	280	98.0

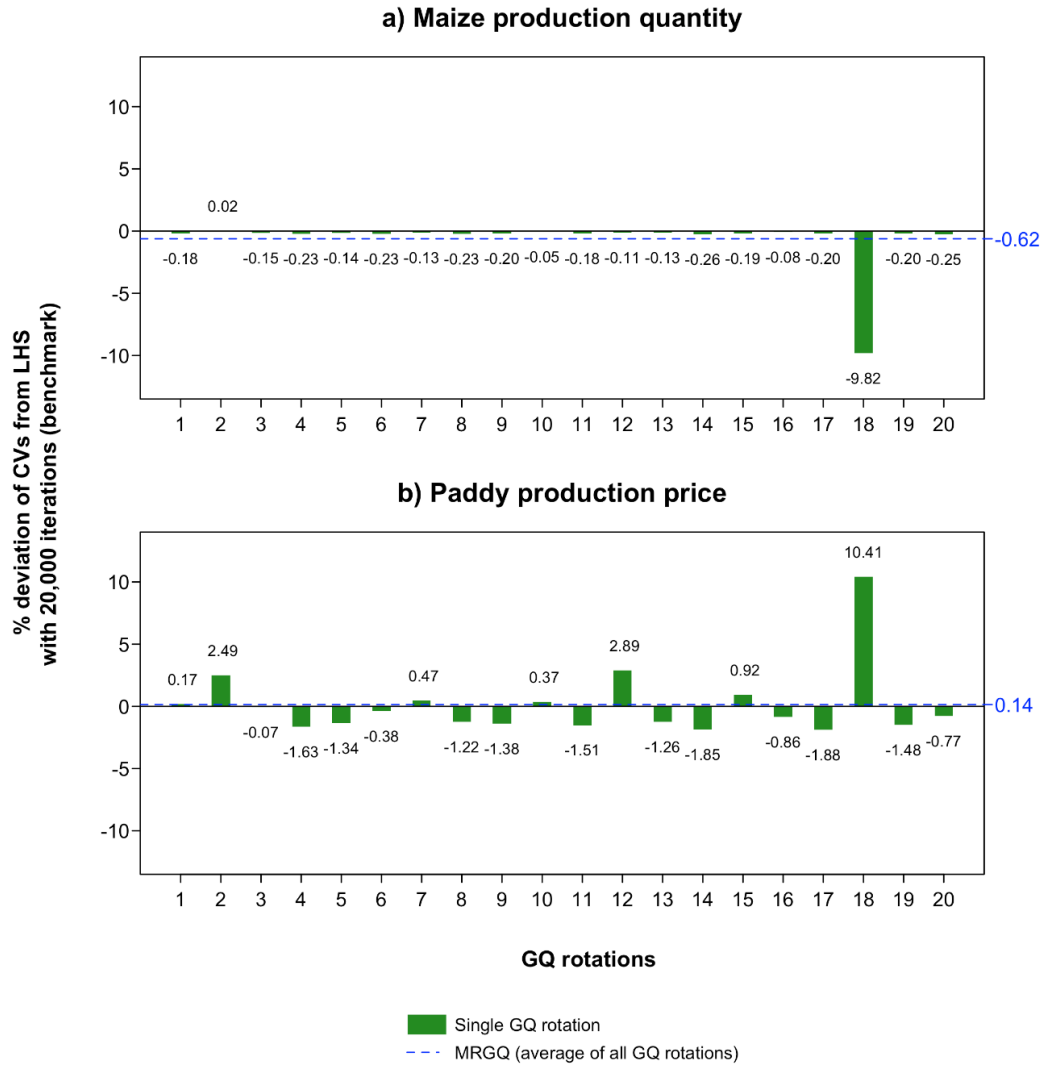

Figure 3.5. Precision of single GQs and MRGQ in the static CGE model (in percent of deviation of the CVs of the results obtained by each GQ family from the benchmark).

Benchmark: LHS with 20,000 iterations. 1-20 (x-axis) are the deviations of the results obtained by 20 randomly generated GQ families; the dashed line is the result obtained by the MRGQ method (*i.e.*, the average of these 20 GQ rotations).

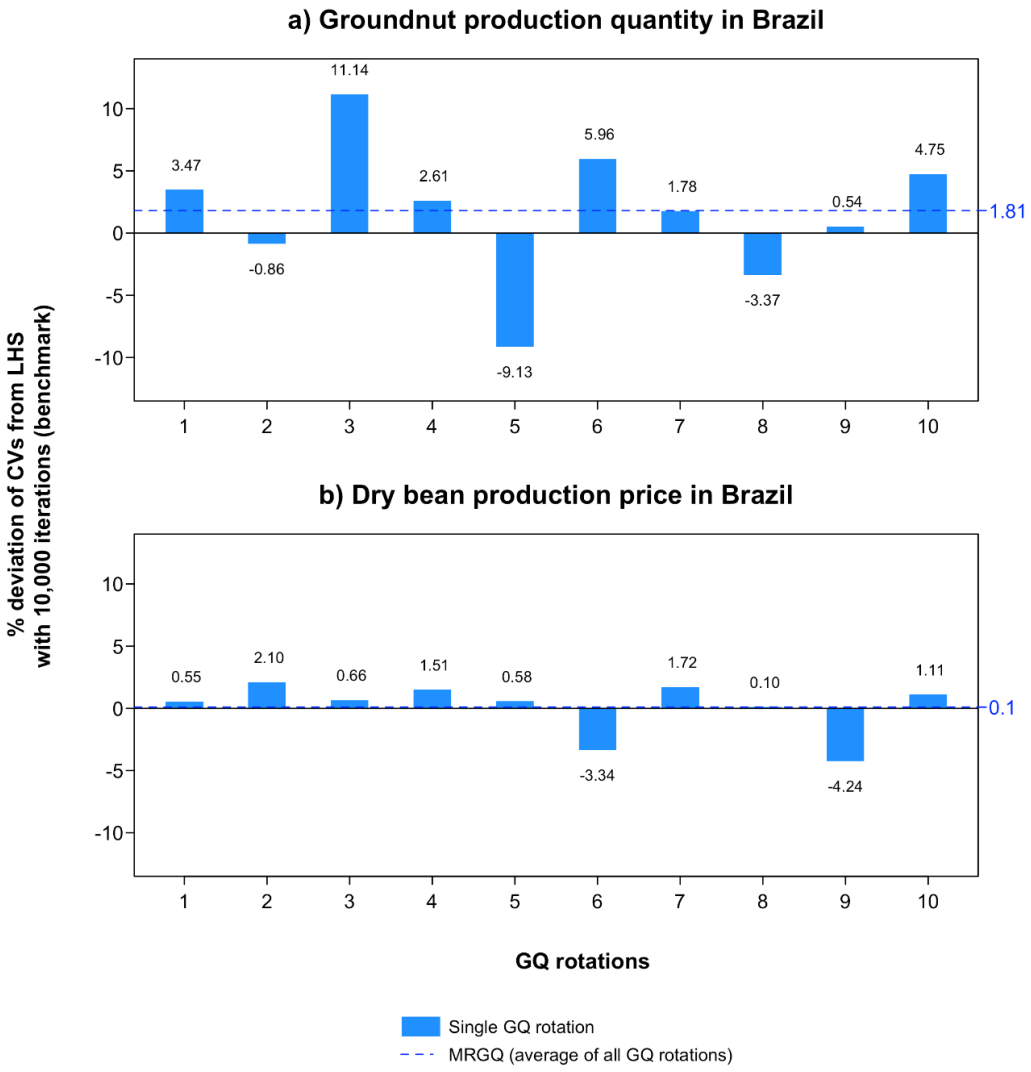

Figure 3.6. Precision of single GQs and MRGQ in the GLOBIOM model (in percent of deviation of the CVs of the results obtained by each GQ family from the benchmark).

Benchmark: LHS with 10,000 iterations. 1-10 (x-axis) are the deviations of the results obtained by ten randomly generated GQ families; the dashed line is the result obtained by the MRGQ method (*i.e.*, the average of these ten GQ rotations).

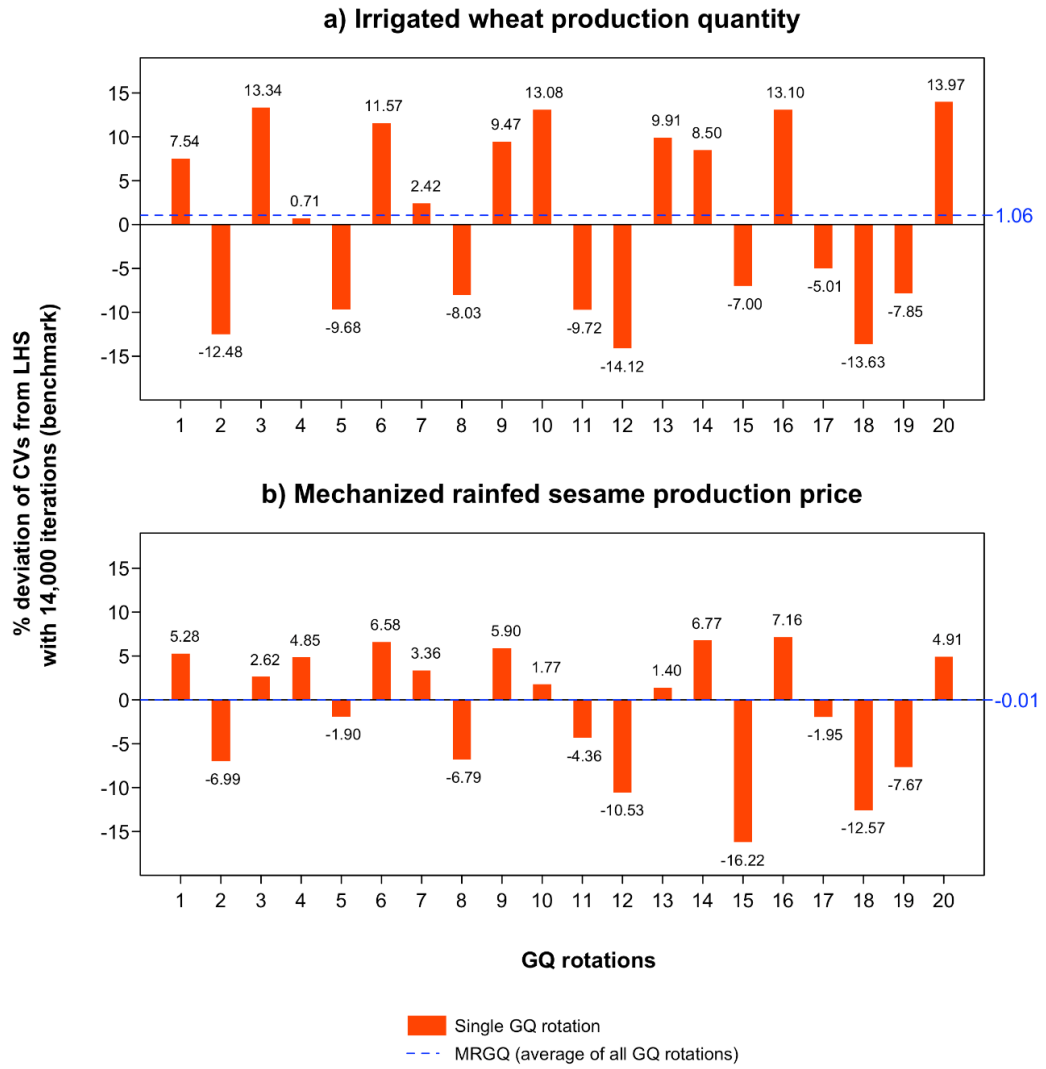

Figure 3.7. Precision of single GQs and MRGQ in the dynamic CGE model (in percent of deviation of the CVs of the results obtained by each GQ family from the benchmark).

Benchmark: LHS with 14,000 iterations. 1-20 (x-axis) are the deviations of the results obtained by 20 randomly generated GQ families; the dashed line is the result obtained by the MRGQ method (*i.e.*, the average of these 20 GQ rotations).

In Figures 3.8, 3.9, and 3.10, we present the complete results for all crops, with yields being considered uncertain in the three models. The difference between the minimum/maximum results and the MRGQ results can be considered a measure for evaluating the improvements made by the MRGQ method as compared to the GQ method. In all three models, we observe large deviations in the approximated results

obtained by a single GQ rotation. More specifically, in static CGE, we observe potential inaccuracies ranging from −10% to +1% for production and from −28% to +29% for prices (Figure 3.8). In GLOBIOM, the inaccuracies range from −21% to +11% and from −24% to +14% for production and prices, respectively (Figure 3.9). In the case of dynamic CGE, we observe inaccuracies in production within the range of −63% to +20%. The inaccuracies in prices in dynamic CGE caused by a single GQ range from −82% to +35% (Figure 3.10). In the vast majority of cases, we see substantial improvements in the results when applying the MRGQ. The average deviations in the MRGQ result in production and price changes of +0.04% and −6.00% for static CGE, −0.24% and −1.30% for GLOBIOM, and +0.09% and +0.90% for dynamic CGE, respectively.

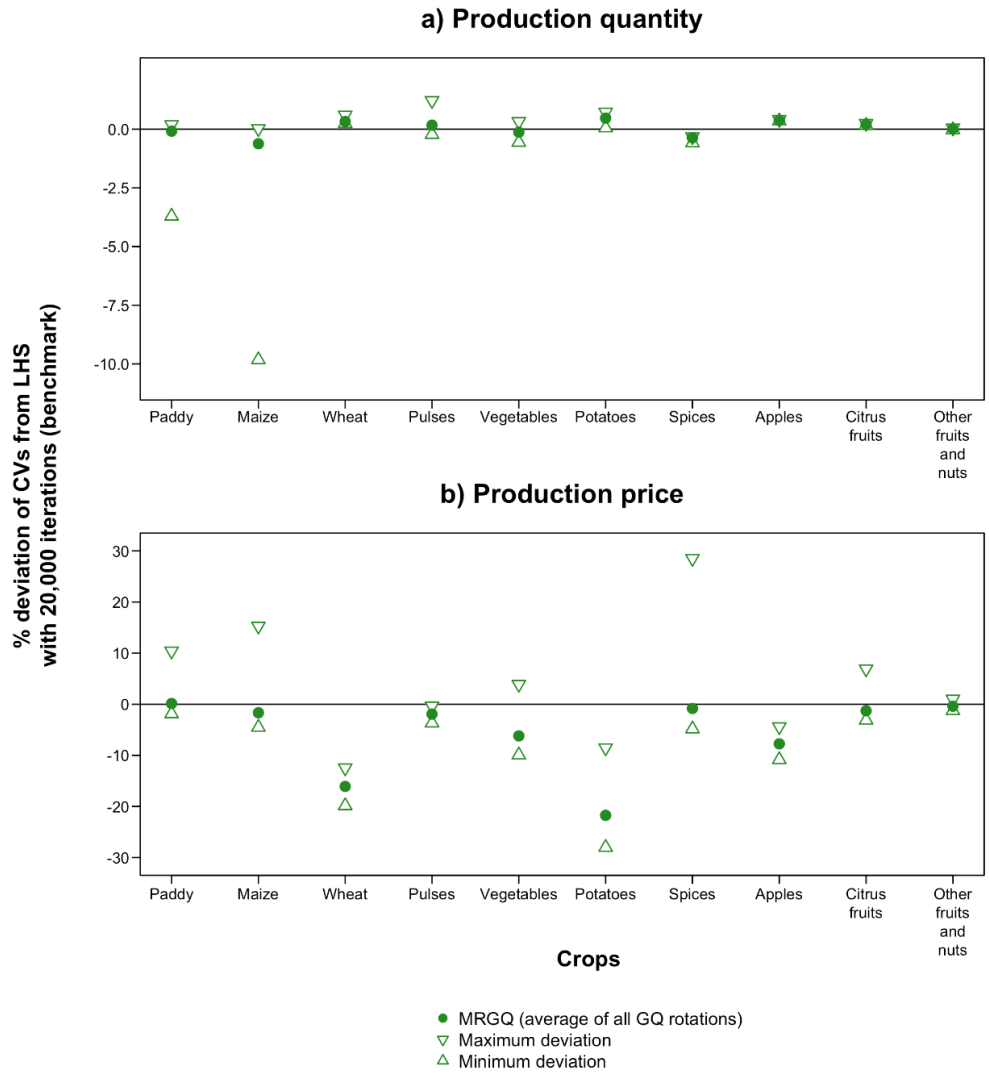

Figure 3.8. Range of deviation of the results produced by single rotations of GQ in the static CGE model.

The deviations are measured in percentage differences of the CVs of the results obtained by each GQ family from the benchmark (LHS with 20,000 iterations). The maximum and minimum deviations for each crop are depicted from 20 randomly generated GQ families. The results obtained by the MRGQ are represented by dots.

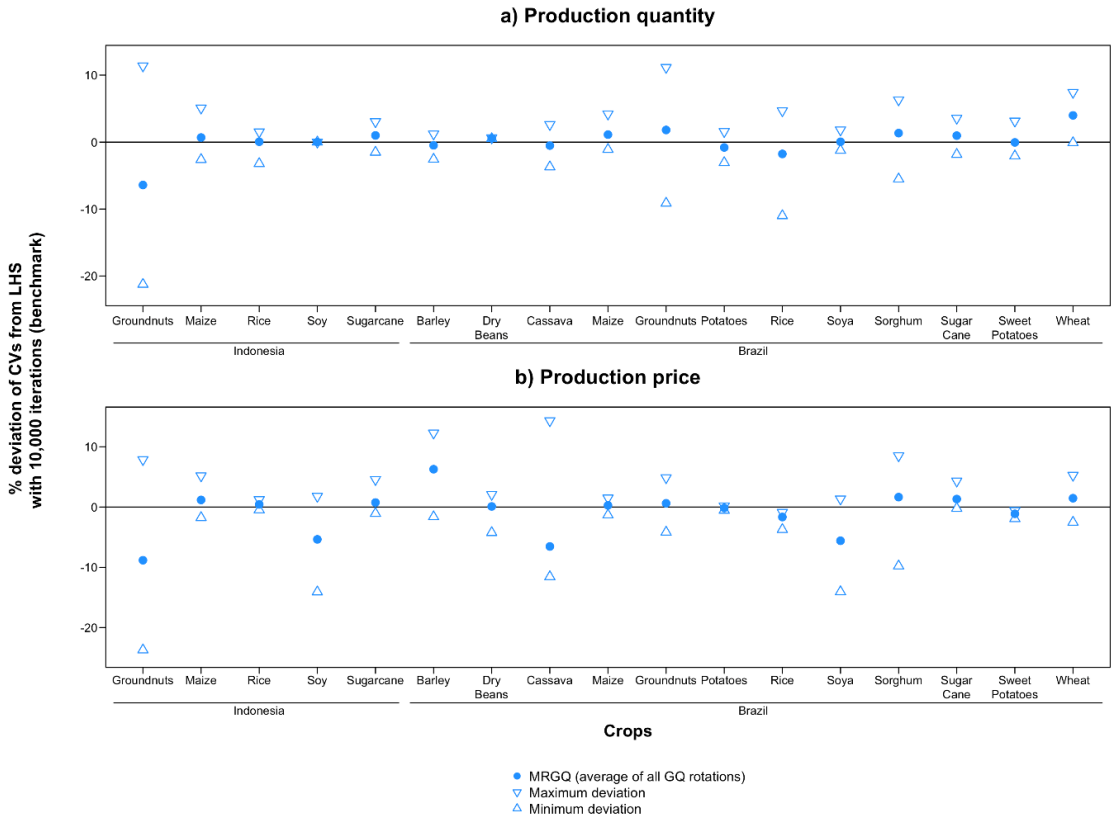

Figure 3.9. Range of deviation of the results produced by single rotations of GQ in the GLOBIOM model.

The deviations are measured in percentage differences of the CVs of the results obtained by each GQ family from the benchmark (LHS with 10,000 iterations). The maximum and minimum deviations for each crop are depicted from ten randomly generated GQ families. The results obtained by the MRGQ are represented by dots.

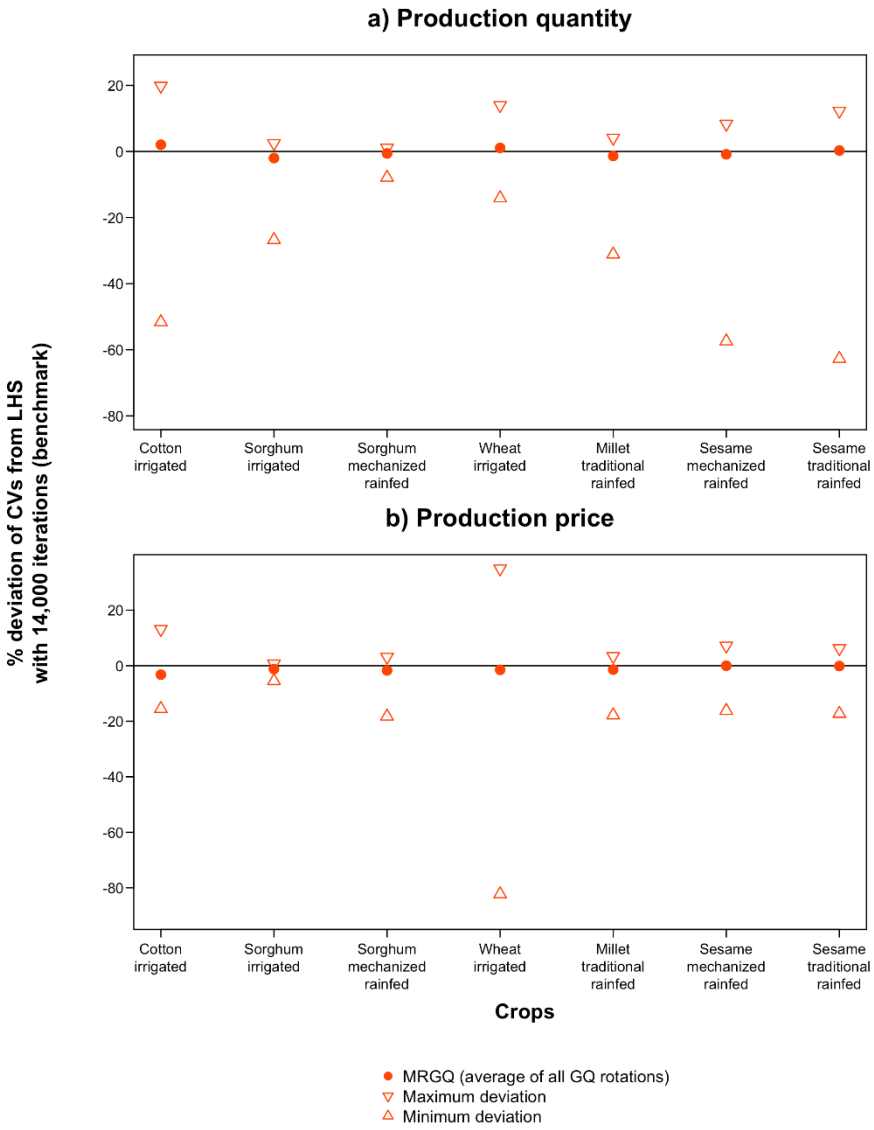

Figure 3.10. Range of deviations in the results produced by single rotations of GQ in the dynamic CGE model.

The deviations are measured in percentage differences of the CVs of the average growth rates of the results obtained by each GQ family from the benchmark during the 2021–2025 period (LHS with 14,000 iterations). The maximum and minimum deviations for each crop are depicted from 20 randomly generated GQ families. The results obtained by the MRGQ are represented by dots.

To observe the differences between the shocks produced by both methods, depicting uncertainties and their impacts on the final results, we also analyze their cumulative distribution functions (CDFs). Figure 3.11 presents a comparison of the CDFs of the shocks generated by the MRGQ method versus the LHS method and the resulting variables from both approaches. As the major difference between the shocks generated by these two methods, unlike the LHS method, the MRGQ method does not capture the tails of the shocks. However, this does not affect the accuracy of the approximation of the central moments of the distribution. According to two-sample t-tests and F-tests, the results obtained from the MRGQ and LHS methods shown in Figure 3.11 do not have significantly significant differences in means or variances at the 99% confidence level (Table 3.2).

Table 3.2. Results of two-sample t-tests and F-tests comparing the means and variances of the output distributions generated by MRGQ and LHS for the results shown in Figure 3.11.

Variable and model	Test	Test value	Critical value (99.00%)	P-value	Note
Paddy prices generated by MRGQ and LHS in static CGE	Two-Sample t-Test	0.01	2.82	0.990	*a*
	F-Test	1.01	1.17	0.461	*b*
Groundnut production in Brazil by MRGQ and LHS in GLOBIOM	Two-Sample t-Test	0.05	2.82	0.960	*a*
	F-Test	1.04	1.19	0.300	*b*
Average mechanized rain-fed sesame prices by MRGQ and LHS in dynamic CGE	Two-Sample t-Test	-0.23	2.83	0.820	*a*
	F-Test	1.08	1.23	0.190	*b*

Note: At a confidence level of 99% we fail to reject H0 in which a) means and b) variances are equal.

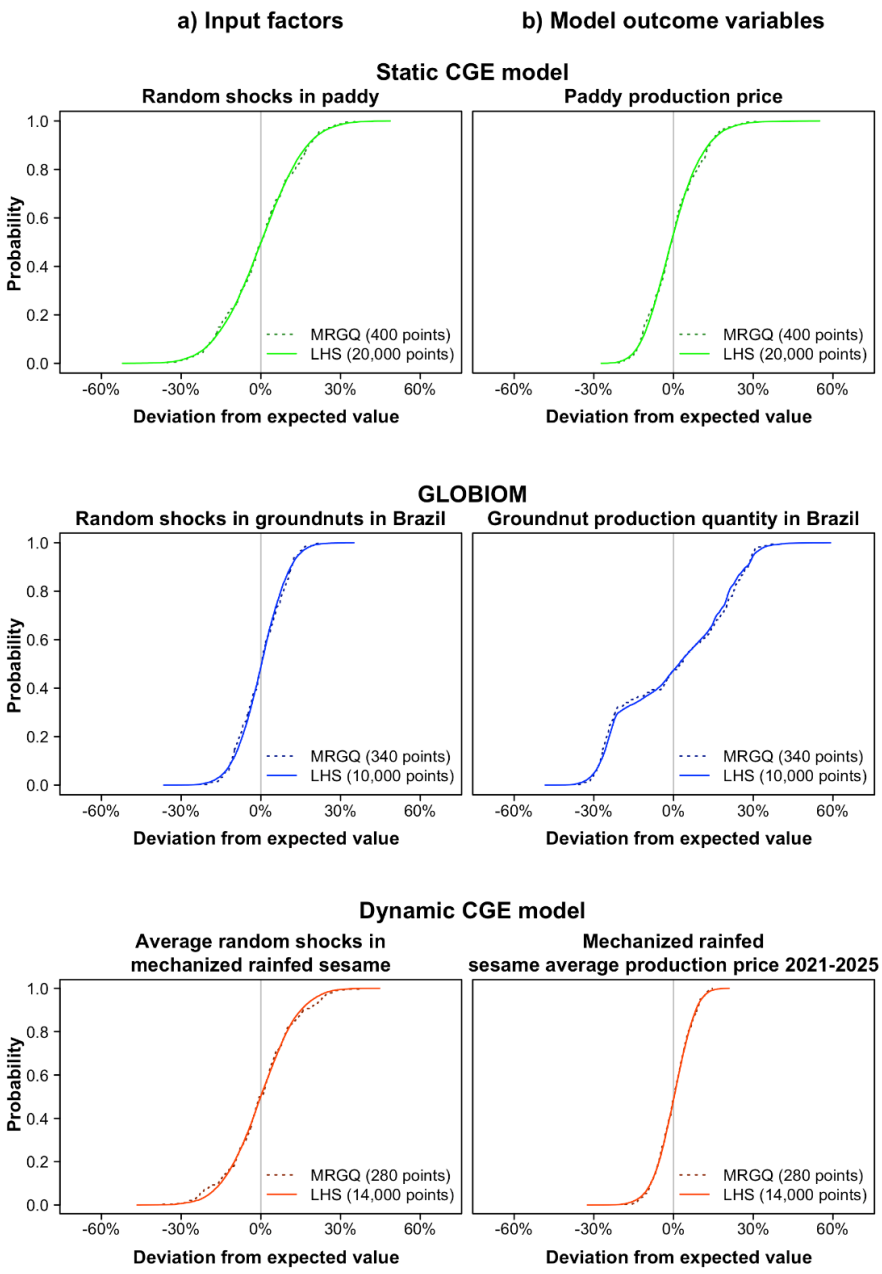

Figure 3.11. CDFs of the uncertain input factors and of the results obtained based on the simulation models comparing LHS and MRGQ.

The CDFs on the right-hand side indicate the results obtained from the simulation models after plugging in the uncertain input factors presented on the left-hand side. The respective number of model runs for each method is indicated in the legends.

Table 3.3 presents the differences between the LHS method and the proposed novel MRGQ approach in terms of the computational and data management requirements. Owing to the modest computational requirements of static CGE, we manage to obtain a benchmark with a relatively short solving time and a small results file. However, solving the same model with the MRGQ method (using 400 iterations) is much faster, requiring only 8% of the computational time and consuming 3% of the computational space as that used by the LHS method.

Of these three models, GLOBIOM is the computationally most burdensome model to solve using the LHS approach. Solving the GLOBIOM model 10,000 times requires 2,500 computer-hours. To produce reliable results, the MRGQ can solve the model using only 340 iterations, which requires only 3% of both the running time and disk space used in the LHS method. Note that the model is run for only one time step. Each additional time step increases the amount of effort proportionally.

In the case of dynamic CGE, a difficulty arises from its recursive-dynamic setup. The original model is set up to project the time interval of 2018–2050. However, to obtain the benchmark results, we must shorten the interval to 2018–2025. Generating a benchmark for a single scenario requires 84 computer hours, and similar to GLOBIOM, dynamic CGE produces a results file of more than 28 GB in size. By contrast, solving the same model with the MRGQ method (using 280 iterations) requires only 6% of the running time and 9% of the disk space consumed by the LHS method, which will allow such an analysis on a single standard equipped notebook.

Table 3.3. Computational effort for MRGQ and LHS in three simulation models

	LHS		MRGQ			
	Size of results file in GB	Model run time (in computer-hours)	Size of results file in GB	Reduction in the size of results file (percentage of reduction from LHS)	Model run time (in computer-hours)	Reduction in model run time (percentage of reduction from LHS)
Static CGE	0.9	9.0	0.03 (20 rotations)	96.7%	0.7	92.2%
GLOBIOM	70.0	2,500	2.36 (10 rotations)	96.6%	160.0	96.6%
Dynamic CGE	28.0	84.0	2.60 (20 rotations)	90.7%	5.0	94.0%

3.7. Discussion

In this chapter, we introduce a novel approach to SSA/UA targeting large-scale simulation models with computational restrictions. The proposed MRGQ method is based on the degree 3 quadrature formulae by Stroud (1957) and incorporates a novel technique to reduce the approximation error, which not only avoids computationally burdensome probabilistic approaches but also offers an approximation quality that is comparable with approaches requiring extremely large sample sizes.

We test the proposed approach on three large-scale simulation models addressing agro-environmental systems, namely, a comparative static CGE model applied to Bhutan (static CGE), a global PE model (GLOBIOM), and a recursive dynamic CGE model applied to the Sudan (dynamic CGE), when considering 10, 17, and 7 uncertain input factors, respectively. To evaluate the accuracy of the results produced by the proposed approach, we generate a benchmark using a probabilistic approach, that is, LHS, with a converged sample size. To reach convergence, we follow the approach by Yang (2011) and gradually increased the sample size until the percent of deviation of the results, compared to those of the previous sample size, remain within the interval of [-1%, +1%].

The convergence criterion is satisfied at 20,000 and 14,000 iterations for the static CGE and dynamic CGE models, respectively, whereas for GLOBIOM, we reach the available computational limit at 10,000 iterations with most of the variables satisfying the convergence criterion. These sample sizes are realized by gradually increasing the number of iterations to reach the stop criterion, thus determining the minimum required sample size in each case. For a fair comparison, the resources required to solve the models and analyze the results with smaller sample sizes would certainly have to be

added to the LHS approach shown in Table 3 because such steps will be needed to determine the sample sizes required for convergence. This will substantially increase the relative advantages of the MRGQ approach. However, to the best of our knowledge, there is no established procedure for determining the starting number of iterations or steps for increasing this number. Hence, we refrained from performing such steps. It is worth noting that many studies applying MC-based approaches to SSA/UA in large-scale simulation models rarely show any convergence because of the computational burden involved (Yang 2011; Sarrazin et al. 2016). Instead, they select one sample size that fits the available computational capacities and assume that the approximations produced match the desired quality (Valin et al. 2015; Villoria and Preckel 2017; Mary et al. 2018).

Depending on the context of its application, there are two potential limitations of the MRGQ method. First, MRGQ do not capture the tails of the distributions because of the restricted sampling interval of Stroud's formulae (see Section 3.3). However, as presented in Table 3.2, this restriction does not limit the MRGQ method to approximate the true distribution with a 99% significance interval. The failure to capture the tails can be seen as both a disadvantage and an advantage. On one hand, the inability of MRGQ to depict the tails of the distributions (*i.e.*, the effects of rare occurrences) can be viewed as a disadvantage if researchers are particularly interested in studying the impacts of extremes. In this case, we suggest implementing MRGQ along with the broader sampling approach proposed by Preckel et al. (2011). This approach allows the sampling intervals of GQ to be widened by the desired expansion factor. On the other hand, many simulation models are unable to handle large shocks to the system well. Owing to technical model constraints, the systems operate far from their region of

calibration and thus far from the sound empirical foundation of the parameters. Therefore, when using probabilistic approaches, researchers often truncate the distribution of the shocks (Hertel et al. 2010; OECD/FAO 2011; Burrell and Nii-Naate 2013), which may result in an inaccurate approximation of the central moments of the results. In such a case, the MRGQ approach is the most suitable method for approximating the central moments of the results without losing information abou the input uncertainty.

As a second limitation, the MRGQ method is restricted to approximating symmetric distributions. The central idea of MRGQ, however, can also be applied to non-symmetric distributions. To this end, we suggest extending the MRGQ approach to depict asymmetric regions using the method developed by DeVuyst and Preckel (2007) for GQ.

3.8. Conclusions

This chapter describes the potential benefits of GQ as an efficient approach to UA in large-scale simulation models. It also shows the limits of traditional GQ approaches because they may generate approximations of significantly lower quality than those generated by traditional probabilistic approaches. Therefore, we develop and test a novel MRGQ method, which overcomes the problem of insufficient accuracy of traditional GQ approaches. Applying MRGQ in three different simulation models reveals two distinct advantages compared to probabilistic approaches. First, the MRGQ method requires a considerably smaller number of iterations when conducting a UA. This is particularly relevant for large-scale or dynamic simulation models and cases in which many variables or simulations need to be analyzed. Second, it produces highly accurate results with considerably lower computational and data management costs.

The MRGQ method allows a systematic UA with high-quality outcomes in large-scale simulation models to be conducted, even in cases where probabilistic approaches become infeasible because of the sample sizes and boundaries required for the computational capacity.

The demand for an efficient and robust approach to conducting UA, as offered by MRGQ, is likely to increase with the ever-expanding size and scope of the simulation models. Despite the rapid growth of computational capacities, the computational requirements in the era of "big data" require more efficient methods.

The proposed approach is successfully tested using three different simulation models integrating uncertainty in various ways. This suggests that the MRGQ method has a high potential as a resource-efficient and highly accurate means of UA in a wide range of large-scale simulation models analyzing the uncertainty of model parameters, exogenous variables, or shocks.

Although the successful application of the MRGQ method in the three case studies shows its advantages in terms of resource (computational and data management) requirements compared to probabilistic approaches, open questions remain. Future research may generate a better understanding of the optimal number of random rotations required to reach a desired accuracy level, given the specific model characteristics. Moreover, research is needed to investigate the factors affecting the quality of GQ points produced by a single rotation of Stroud's octahedron.

Chapter 4

Stochastic simulation with informed rotations of Gaussian quadratures

Chapter 4

4. Stochastic simulation with informed rotations of Gaussian quadratures[8]

4.1. Abstract

Given the fast growth of available computational capacities and the increasing complexity of simulation models addressing agro-environmental issues, uncertainty analysis using stochastic techniques has become a standard modeling practice. However, conventional uncertainty/sensitivity analysis methods are either computationally demanding (Monte Carlo-based methods) or produce results with varying quality (Gaussian quadratures). In this chapter, we present a computationally inexpensive and reliable uncertainty analysis method for simulation models named informed rotations of Gaussian quadratures (IRGQ). We also provide a linear programming model that generates IRGQ points based on the required input data. The results demonstrate that this method is able to produce approximations that are close to the estimated benchmarks at low computational costs. The method is tested in three different simulation models using different input data in order to demonstrate the independence of the proposed method on specific model types and data structures. This is a methodological study for practitioners rather than theorists.

[8] This chapter is based on and in large parts identical with Stepanyan et al. (2020).

4.2. Introduction

In recent decades, the increases in available computational power and speed have led to simulation models – especially those addressing agricultural and environmental issues – becoming more detailed and complex. Complexity can be represented by the number of parameters and variables that a model incorporates (Razavi and Gupta 2016). By increasing the number of parameters and variables, however, the degree of uncertainty of the model associated with each parameter and variable also increases. In order to account for this uncertainty, the application of uncertainty (UA) and/or sensitivity analysis (SA) techniques, mostly by incorporating stochastic elements into the simulation model, has become a standard modeling practice (Artavia et al. 2015). Many well-established and widely used economic simulation models have already adopted stochastic modeling approaches to cope with the model uncertainty related to model parameters, data and shocks. For example, the AGLINK-COSIMO model, which is a widely used partial equilibrium (PE) model to analyze the supply and demand of global agricultural markets, applies the well-known Monte Carlo (MC)-based method called Latin hypercube sampling (LHS) for stochastic applications (OECD/FAO 2015). The GLOBIOM model, which is also a PE model used by the International Institute for Applied Systems Analysis (Havlík et al. 2011; Havlík et al. 2014) to analyze the competition for land between agricultural, forestry and bioenergy sectors globally, applies the MC approach (Ermolieva et al. 2016; Fuss et al. 2015; Valin et al. 2015). However, there have been some recent attempts to reduce the computational costs of solving the stochastic version of the model by adopting a more computationally efficient method known as Gaussian quadratures (GQs) (Stepanyan 2018a). The global trade analysis project (GTAP) model is one of the most commonly used general equilibrium models (CGE) with global coverage (Hertel 1997). The standard approach

to stochastic modeling in the GTAP model is via GQs, and this approach is considered to be an efficient uncertainty quantification method (Verma et al. 2011; Thurlow et al. 2012; Villoria et al. 2013). The GQ approach is also applied in the European simulation model (ESIM), an established PE model designed to analyze medium-term developments in EU agricultural markets (Artavia et al. 2015). However, Artavia et al. (2015) discovered that depending on the rotation of Stroud's octahedron (*i.e.,* the arrangement of the coordinates of Stroud's generalized n-octahedron) used to generate the GQ sampling points, the quality of the approximations varies considerably. These results have been confirmed by two other studies. Villoria and Preckel (2017) confirmed that in certain cases, the results generated by the GQ method have large deviations from the results obtained by the MC method using the GTAP model. Stepanyan et al. (2019b) demonstrated similar effects in three other simulation models and proposed a novel approach named multiple rotations of Gaussian quadratures (MRGQ) that considerably reduces approximation errors by moderately increasing the sample size.

In this chapter, we address the open questions from Artavia et al. (2015) regarding why the quality of the approximation depends on the choice of the rotation and how to choose rotations that provide better results. To answer these questions, a novel approach named informed rotations of Gaussian quadratures (IRGQ) is presented. To demonstrate the proposed approach, we use the same simulation model, data and covariance structure as Artavia et al. (2015). In order to avoid the dependence on a certain model type and covariance structure of the stochastic variables, we also demonstrate the method based on two other simulation models, namely, a recursive-dynamic single-country CGE model for the Sudan (Diao and Thurlow 2012) and a global PE model integrating agricultural, bioenergy and forestry sectors (Havlík et al.

2011; Havlík et al. 2014). In addition to this study, we provide an LP model implemented in Wolfram Mathematica that, given the necessary input data, such as the covariance matrix of the stochastic input factors, their base values, and the number of desired families of points, generates IRGQ points. The generated IRGQ points can be exogenously incorporated into any simulation model for stochastic analysis.

The remainder of this chapter is organized as follows. Section 4.3 provides a literature review covering the current practices of UA/SA in simulation models, Section 4.4 introduces the theoretical background of Gaussian quadratures, Sections 4.5 and 4.6 explain the theory behind the proposed method and the validation procedure, respectively, and Section 4.7 presents the results obtained using the proposed method for three different simulation models. Finally, Section 4.8 offers a discussion and conclusions.

4.3. Uncertainty and sensitivity analysis in simulation models

UA or SA methods can be categorized into local or global (Liang et al. 2017). Local methods consider the uncertainty of the model output against variations of a single input factor (Pianosi et al. 2016). Therefore, the shortcomings of the methods in this group are that they do not consider the interactions among the uncertainties of the input factors and therefore only provide a limited view of model uncertainty. Global methods evaluate input uncertainty over the entire range of the input space by varying all input factors simultaneously (Matott et al. 2009). These methods allow for a more comprehensive depiction of the model uncertainty (Saltelli and Annoni 2010). Saltelli et al. (2019) claim that SA/UA should always be based on global methods in order to adequately represent models with nonlinearities. According to Douglas-Smith et al. (2020), the number of studies in the field of environmental science that apply UA or

SA methods has increased fivefold in the last two decades. However, the number of studies introducing new uncertainty quantification methods has hardly changed. Razavi and Gupta (2016) claim that the conventional approaches to UA/SA suffer from poor computational efficiency in terms of computational and data management efforts to produce statistically robust and stable results. Amid the increasing use of different UA/SA techniques in economic simulation models, the quality of the results produced by these methods is often not considered by users. When working with MC-based methods, the quality of the model results can be guaranteed by convergence evaluations. This is a method used to determine the appropriate MC sample size for a given problem. Yang (2011) suggests two methods for monitoring the convergence of MC-based approaches. The first method is based on the central limit theorem and suggests solving the model by gradually increasing the MC sample size and comparing the coefficients of variation (CVs) of the results of interest obtained by each sample size. With this method, convergence is achieved if there are no significant changes in the CVs when increasing the sample size. In economic simulation models, this is a widely used method for convergence evaluations, such as in, e.g., Artavia et al. (2015), Stepanyan et al. (2019b) and Chatzivasileiadis (2018). The second convergence evaluation method is based on bootstrapping techniques and, according to Yang (2011), is not very commonly used in agro-environmental simulation modeling. Nonetheless, the application of MC-based methods in large-scale simulation models often becomes impractical in terms of the computational effort (Kompas and van Ha 2019). Arndt (1996) is the pioneering study that introduced Stroud's (1957) order 3 GQ in an economic simulation model, namely, in the GTAP model, as an efficient method for stochastic modeling. The efficiency of this method is outstanding due to the small number of model runs required to solve a stochastic problem. More specifically, it

requires only 2n points, where n is the number of stochastic input factors. Several articles have discussed the quality of the results produced by the GQ method. Preckel et al. (2011b) address the question of whether using different linear transformation methods to incorporate the correlation of stochastic input factors into stochastic shocks affects the quality of the results. To answer this, they evaluate two linear transformation methods, namely, the Cholesky factorization method and the eigensystem decomposition method, using three CGE models with different levels of aggregation and with different covariance structures. They conclude that the selection of a particular linear transformation method is not crucial for the quality of the results. Preckel et al. (2011a) explore whether the limited sampling interval of the GQ method affects the quality of the results and, if so, under which model conditions this impact is significant. Moreover, they suggest a method of expanding the sampling interval of the method using a desired expansion factor that doubles the number of required model runs. Their findings suggest that the sampling breadth is important for highly nonlinear models. Artavia et al. (2015) examine whether the rotations of Stroud's octahedron used to generate GQ points affect the quality of the results using a global PE model named ESIM. They find that the quality of the approximation indeed depends on the choice of the rotation. This finding has generated discussions about the appropriateness of the GQ method and options to reduce the approximation error of the method. Villoria and Preckel (2017) evaluate the quality of GQ-based results compared to MC-based results in the GTAP model and discover large differences in the first three moments of the probability distributions of the results. Stepanyan et al. (2019b) suggest a method called MRGQ for decreasing the approximation error of the GQ. The method was successfully tested in three very different models in order to avoid the biases created by specific models and correlation structures. It was shown that the method decreases the

approximation error considerably while keeping the number of required model runs low compared to MC-based methods. However, the questions of what factors affect the quality of the rotation and how to choose the rotations generating low approximation errors have not yet been answered.

4.4. Theoretical background on Gaussian quadratures

The incorporation of stochastic elements into a simulation model turns it into a problem of numerical integration that can be approximately solved using numerical methods. For example, the calculation of the first two moments (the expected value and variance) of a function *f(x)* with random inputs drawn from a given probability density function *g(x)* describing the uncertainty of *x* on an interval [a, b] will yield the following equations:

$$E(f(x)) = \int_a^b f(x)g(x)dx, \tag{4.1}$$

$$Var(f(x)) = E((f(x) - E(f(x)))^2) = \int_a^b (f(x) - E(f(x)))^2 g(x)dx. \tag{4.2}$$

Consequently, since those equations cannot be evaluated analytically, they should be approximated numerically using weighted sums of the evaluations of these integrands:

$$\tilde{E}(f(x)) = \sum_{i=1}^{n} f(x_i)w_i, \tag{4.3}$$

$$\tilde{Var}(f(x)) = \sum_{i=1}^{n} (f(x_i) - \tilde{E}(f(x)))^2 w_i. \tag{4.4}$$

Here, x_i are the n points chosen from the integration space at which the function *f(x)* is being evaluated, and w_i are the weights associated with each point. This approach can easily be extended to multivariate cases. For example, the form of the equation to

approximate the expected value of the function *f(x)* will remain the same as in equation (4.1) with the exception that *x* will be regarded as a vector now and the integration will occur over the whole Euclidean space (R^d):

$$E(f(\vec{x})) = \int_{R^d} f(\vec{x})g(\vec{x})d\vec{x} \tag{4.5}$$

One of the most famous and widely applied methods for drawing these points from a probability density function and assigning weights is the Monte Carlo method (Metropolis and Ulam 1949), which suggests randomly selecting equally weighted points from a probability distribution. Thus, according to the law of large numbers, the approximation will be close to the true value if the number of random draws is sufficiently large. However, this often creates problems in terms of computational requirements when applied to large-scale simulation models. Haber (1970) expresses the slow speed of convergence of this method by saying the following: "… to get one additional decimal place of accuracy it is necessary to increase the number of points by a factor of one hundred". Moreover, Haber (1970) demonstrates that to achieve an accuracy level of 1%, the number of random points should range from 40,000 to 100,000. However, the advantage of this method is that the quality of the approximations is independent of the dimensionality or the nonlinearity of the problem and of the smoothness of the integrand (Schürer 2003).

Another widely used method, called GQ, is very attractive due to its low computational requirements. This type of method is clearly more efficient and accurate than the MC-based approaches in the case of smooth integrands (Schürer 2001). Here, we are referring to the GQs of degree 3 by Stroud (1957) who proved that a necessary and sufficient condition for 2n points to form an equally weighted numerical integration formula of degree 3 for symmetrical regions, where n is the number of stochastic

variables (*i.e.,* the dimension of the problem), is that these 2n points are the vertices of an n-dimensional regular octahedron of the properly chosen size that has the same centroid as the region of integration. If the region is an n-cube, he suggested using the vertices with the following positions relative to the centroid in order to ensure that the vertices still lie inside the cube. For the k^{th} quadrature point $\Gamma_k = (\gamma_{k1}, \gamma_{k2,\ldots}, \gamma_{kn})$, where k=1,…,2n:

$$\gamma_{k,2j-1} = \sqrt{\frac{2}{3}} \cos\left(\frac{(2j-1)k\pi}{n}\right), \tag{4.6}$$

$$\gamma_{k,2j} = \sqrt{\frac{2}{3}} \sin\left(\frac{(2j-1)k\pi}{n}\right), \tag{4.7}$$

for $j = 1,\ldots,[n/2]$, where $[n/2]$ is the greatest integer not exceeding n/2. In addition, if n is odd:

$$\gamma_{k,n} = \frac{(-1)^k}{\sqrt{3}}. \tag{4.8}$$

Arndt (1996) applied Stroud's (1957) result to the case of the integral over all of R^d, weighted with the standard normal distributions, which became a standard approach of systematic sensitivity analysis in the GTAP model. This yielded the following formulae. For the k^{th} quadrature point $\Gamma_k = \left(\gamma_{k,1}, \gamma_{k,2}, \ldots, \gamma_{k,n}\right)$, where k = 1, …, 2n:

$$\gamma_{k,2j-1} = \sqrt{2} \cos\left(\frac{(2j-1)k\pi}{n}\right), \tag{4.9}$$

$$\gamma_{k,2j} = \sqrt{2} \sin\left(\frac{(2j-1)k\pi}{n}\right), \tag{4.10}$$

for $j = 1,\ldots,[n/2]$, where $[n/2]$ is the greatest integer not exceeding n/2. In addition, if n is odd:

$$\gamma_{k,n} = (-I)^k . \tag{4.11}$$

The details can be found, e.g., in Stepanyan et al. (2019b).

In order to adapt these nodes to the case of a multivariate normal distribution with expected values $\vec{\mu}$ and covariance matrix Σ, we first need to multiply the sampling points generated by formulae (4.9) – (4.11) by a square matrix A satisfying $\Sigma = AA^T$. Artavia et al. (2015) suggest several methods for obtaining A from Σ, namely, the diagonalization method (referred to as eigensystem decomposition in this article), the Cholesky decomposition, and the reverse Cholesky decomposition. The final GQ points are then obtained as follows:

$$\vec{GQ}_k = A \cdot \vec{\Gamma}_k + \vec{\mu}, \tag{4.12}$$

where $\vec{\mu}$ is the vector of the base values of the stochastic parameters.

4.5. Identification of good rotations: theory

As demonstrated in Chapter 3, for an n-dimensional stochastic modeling problem, it is possible to obtain n! families of GQ points generated by the permutations of the n coordinates of Stroud's generalized n-octahedron, where each family consists of 2n points. However, it is also shown in three different simulation models that those families of GQ points yield different quality approximation results due to the disposition of the GQ points. Thus, extensive computations suggested that the relative positions of the quadrature points within a family of GQ points have a strong influence on the quality of the results. Furthermore, following the method proposed by Campolongo et al. (2007) that suggests improving the elementary effects method

(Morris 1991) by maximizing the dispersion of the sampling points in the input space[9], from all the possible permutations (n!), we select the ones for which the nodes in the generated GQ families are spread out the most. Therefore, we introduce the following terminology: the dispersion of a GQ family is the minimum of the distances between any two nodes of the family, *i.e.*,

$$disp(\vec{GQ}_k) = \min_{j \neq i} \left\| x_j - x_i \right\|. \tag{4.13}$$

As the numerical experiments show, on average, GQ families with a larger dispersion perform better than GQ families with a smaller dispersion. Therefore, among all the generated GQ families, we select the ones with the maximum dispersion, *i.e.*, $max(disp(\vec{GQ}_k))$.

To illustrate the idea, Figure 4.1 shows the situation in two dimensions, where a family of GQ points consists of the endpoints of conjugate diameters of the ellipse. In the illustrated examples, the GQ points shown in Figure 4.1c promise better quality results than those in Figure 4.1a and Figure 4.1b according to the method proposed above.

[9] The dispersion is maximized by selecting the samples with the maximum distance between a couple of trajectories. Interested readers are referred to Campolongo et al. (2007).

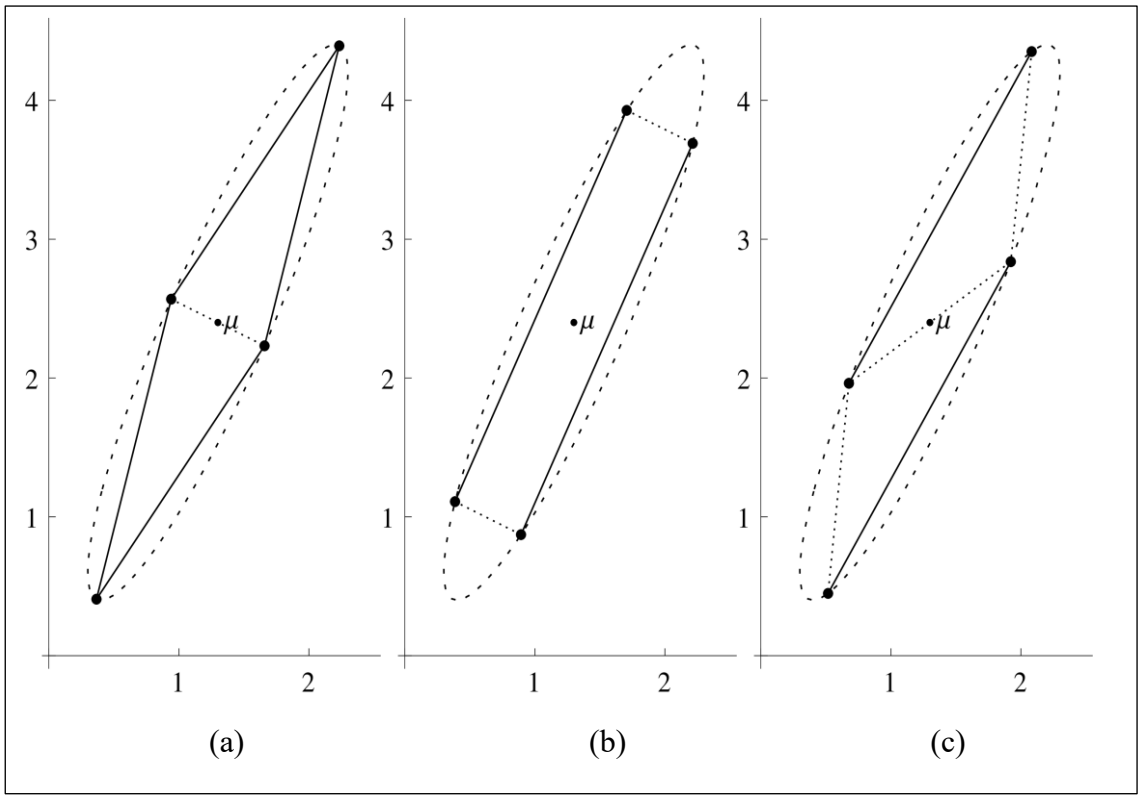

Figure 4.1. Three examples of the disposition of GQ points (black dots) in R2 (two-dimensional space). Here, μ is the centroid of the ellipse, and the dotted lines indicate the shortest connection between pairs of points.

Similarly, Figure 4.2 shows two examples of GQ families in a three-dimensional space (R^3). Again, one can observe that the dispersion of the GQ points in Figure 4.2a is smaller than that in Figure 4.2b; consequently, according to our proposed method, we expect the GQ points depicted in Figure 4.2a to produce lower quality results than those in Figure 4.2b.

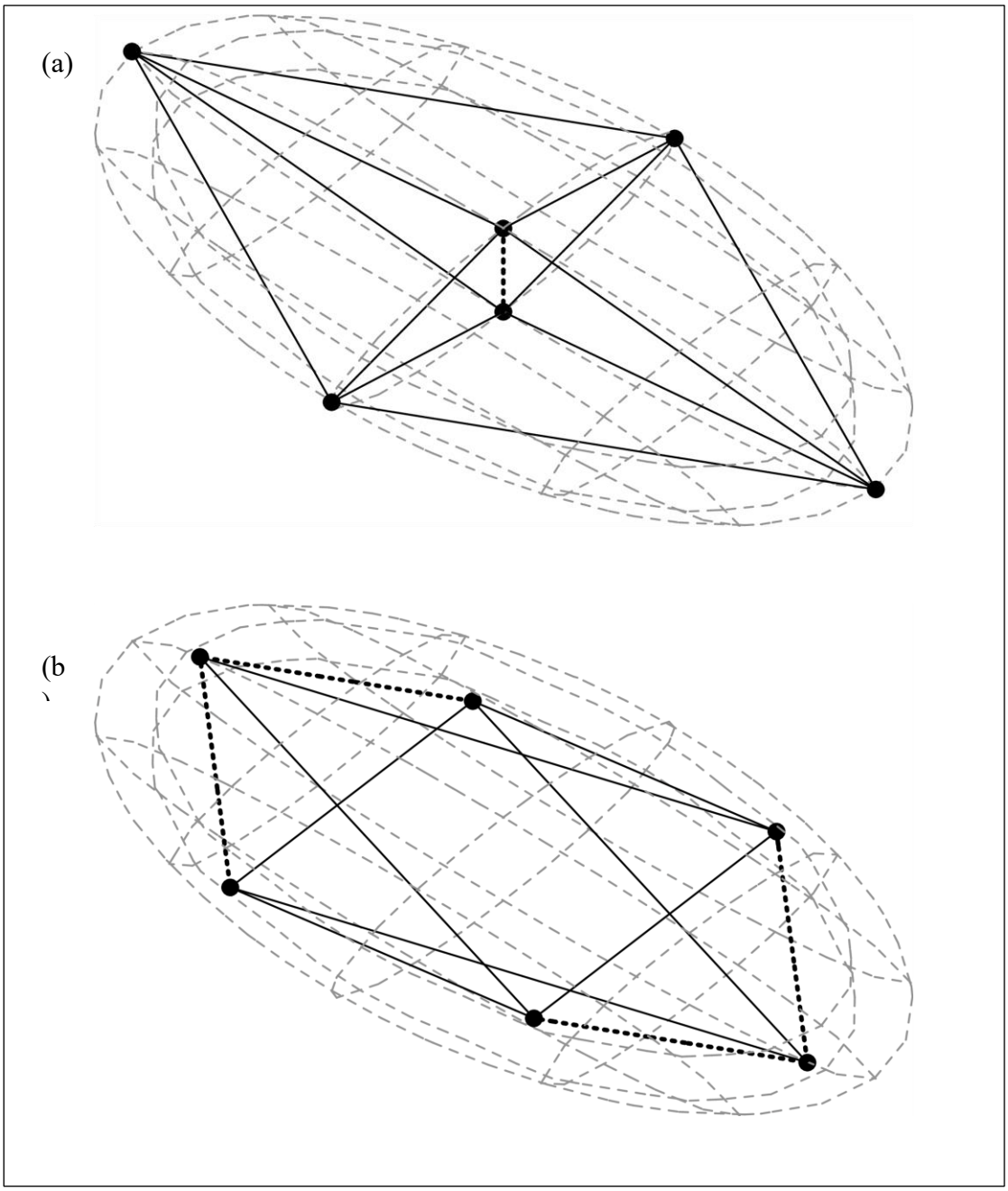

Figure 4.2. Two examples of the disposition of GQ points (black dots) in R3 (three-dimensional space). The dotted lines indicate the shortest connections between pairs of points.

In practical applications, we have to pay heed to the immensely fast growth of n!, which is the number of permutations of n coordinates, *i.e.,* the possible rotations of Stroud's octahedron generated from the permutations of the n coordinates (Stepanyan et al. 2019b). Thus, if the dimensionality of the problem is beyond the available

computational capacity, we suggest selecting a sufficiently large sample of randomly generated GQ families and choosing the ones with the maximum dispersion of points within this sample. This procedure is elaborated in a more detailed way in the next sections.

4.6. Identification of good rotations: method

4.6.1. Experimental design

As explained in Section 4.5, we adapt the approach proposed by Campolongo et al. (2007) to the GQ method by choosing the families of GQ points that have maximal dispersion. For this purpose, we perform all the possible permutations of the n coordinates of Stroud's n-octahedron and select ten rotations with maximal dispersion and ten rotations with minimal dispersion. Thus, we obtain ten GQ families that presumably will yield better quality results and ten GQ families that will yield poor quality results. However, since we are dealing with three simulation models with different numbers of stochastic variables, *i.e.,* different dimensionalities, we adopt the following strategy. If the dimensionality of the problem is lower than or equal to ten, we generate all the possible GQ families; and from these families, we choose ten with maximal dispersion and ten with minimal dispersion. Whenever the dimensionality of the problem is higher than ten, we randomly select a sample of 10! (= 3,628,800) GQ families and choose the respective GQ families with the desired dispersion from this list. The dimensionalities of the simulation models applied in this study are as follows: the ESIM model has 42 dimensions, the recursive-dynamic CGE model has seven dimensions and the GLOBIOM model has 17 dimensions.

4.6.2. European simulation model (ESIM)

Based on the results from Artavia et al. (2015), we first test our claim on the simulation model and data used in their study. ESIM (Grethe 2012) is a global PE model addressing the production and consumption of agricultural products. In this model version, all the member states of the European Union (EU), Turkey and the US are modeled as individual regions while all the other countries are aggregated and represented as the "Rest of the World (ROW)". In the stochastic version of the model documented in Artavia (2014), the barley, rapeseed and wheat yields are considered stochastic in all regions. Those crops are selected due to their significant importance in the EU. In order to reduce the dimensionality of the problem, the EU member states are grouped according to their production shares and the level of correlation of their yield deviates (Artavia et al. 2015). This grouping yields 42 stochastic variables in total.

Since the focus of the model is mainly on the EU, the production side of the model for all EU member states is represented in a more detailed way than for other countries. Namely, the supply is given as the product of the area and yield:

$$Supply = Area \cdot Yield. \tag{4.14}$$

The stochastic crop yields are modeled with isoelastic functions depending on the intercepts (intyd), producer prices (PP), cost indices for intermediate inputs and labor (indi and indl, respectively), technical progress (tp), and stochastic shocks (stoch):

$$Yield = int\,yd \cdot PP^{elastyd} \cdot indi^{elastyi} \cdot indl^{elastyl} \cdot tp \cdot (1 + stoch), \tag{4.15}$$

where *elastyd* is the own-price elasticity of a yield, *elastyi* is the yield elasticity with respect to intermediate input cost indices, and *elastyl* is the yield elasticity with respect to labor cost indices.

The crop production in the rest of the regions is represented by an isoelastic stochastic supply equation:

$$Supply = int\,sp \cdot \prod_{crops} PP^{elastsp_{crops,crops}} \cdot tp \cdot (1 + stoch), \tag{4.16}$$

where *intsp* is the intercept, and $elastsp_{crops,crops}$ are the own and cross-price elasticities of supply.

The correlation structure of the stochastic variables generated from the historical yield data of the respective crops has been adopted from Artavia et al. (2015).

The quality of the results obtained by the proposed method is evaluated against the benchmarks generated by Artavia et al. (2015). These benchmarks were generated using the Latin hypercube sampling (LHS) method (Helton and Davis 2003), and the appropriate sample sizes were determined using the convergence evaluation method based on the CVs, as suggested by Yang (2011).

4.6.3. Other simulation models

In order to demonstrate the independence of the performance of the method from a particular model type and covariance structure, we tested the proposed approach in two other simulation models, namely, a single-country, recursive-dynamic CGE model (Diao and Thurlow 2012) and a global PE model known as GLOBIOM (Havlík et al. 2011; Havlík et al. 2014).

The economy-wide, recursive-dynamic CGE model (Diao and Thurlow 2012) is linked to the IMPACT modeling system (Robinson et al. 2015). The model is calibrated to the most recent social accounting matrix for the Sudan with multiple sectors, out of which 26 are crop producing (Siddig et al. 2016). The demand for primary factors is governed

by constant elasticity of substitution (CES) functions, and the intermediate input demand is determined by Leontief fixed-coefficient technology functions. Government savings are assumed to be flexible while direct tax rates are fixed. Regarding the external balance, a flexible exchange rate is selected, and foreign savings are fixed. Regarding the savings-investment identity, a fixed share of investment in absolute absorption is assumed, and household saving rates adjust endogenously in a uniform way so as to generate the necessary funds.

The uncertainty of the following crop yields is analyzed: irrigated cotton, irrigated and mechanized rain-fed sorghum, irrigated wheat, irrigated groundnuts, mechanized rain-fed millet, and mechanized and traditional rain-fed sesame. The study is conducted for the time interval 2018 to 2025. Considering the cyclical manner of extreme weather shocks in Sudan (MEDP 2013), which on average occur about every five years, stochastic shocks are applied every fifth year; in this case, they are applied in 2018 and 2023. The estimated benchmarks (obtained using 14,000 MC points) and the covariance structure for this model have been taken from Stepanyan et al. (2019b).

GLOBIOM is a bottom-up, recursive-dynamic PE model with global coverage of the agricultural, bioenergy and forestry sectors (Havlík et al. 2011; Havlík et al. 2014). It is a linear programming model with a spatial equilibrium approach (Takayama and Judge 1971). The market equilibrium for agricultural and forestry products is computed based on a welfare-maximizing objective function subject to resource, technology, demand and policy constraints. The model version used in this study covers 31 regions globally and considers the 18 most important crops in terms of globally harvested quantities. Given the large computational requirements of the model version, we use it in a comparative static framework, starting from a fixed 2010 solution and solving the model only for one time step (2020). We analyze the yield uncertainties of Indonesia

and Brazil. The uncertainty of the following crops is tested in each region: 1) groundnuts, maize, rice, soybeans and sugarcane grown in Indonesia; and 2) barley, groundnuts, sorghum, potatoes, dry beans, rice, wheat, sugarcane, maize, soybeans, cassava and sweet potatoes grown in Brazil. The benchmarks (obtained using 10,000 MC points) and the covariance structure of the stochastic input factors computed by Stepanyan et al. (2019b) are adopted.

4.6.4. LP model for generating IRGQ points

The operational process of the LP model is shown in Figure 4.3. The necessary data for the model to produce IRGQ points are a vector of base values of stochastic parameters $(\vec{\mu})$, a covariance matrix of stochastic parameters (Σ), and the number of GQ families desired (k). In the standard case, k should be set to 1, thus producing 2n GQ points, where n is the number of stochastic input factors. The first stage of the model is to check whether the provided data are consistent, *i.e.,* whether the covariance matrix is positive definite, whether the covariance matrix and the vector of base values have the same dimension, and whether the selected number of GQ families is less than or equal to the maximum attainable number of GQ families ($k \leq n!$). If these conditions are satisfied, the model will start calculating the square matrix A, as explained in Section 4.4, using the eigensystem decomposition method, and then it will generate the Γ matrix of Stroud points using equations (4.9) – (4.11). The next stage is to perform the rotations of Stroud's octahedron, as explained in Section 4.5. Since the number of possible rotations generated by the permutations of the n coordinates, *i.e.,* the number of all the GQ families that may be generated from the given data, is equal to n!, its rate of growth is very fast, which may cause computational problems in higher dimensions. Therefore, if the dimensionality of the problem is less than or equal to ten, the model performs all

possible permutations. If the number of dimensions is larger than ten, the model randomly selects a sample of GQ families generated from 10! random rotations of Stroud's octahedron (a sample consisting of 3,628,800 GQ families). Then, it computes the dispersion of each of the generated GQ families and finally selects k GQ families with maximal dispersion.

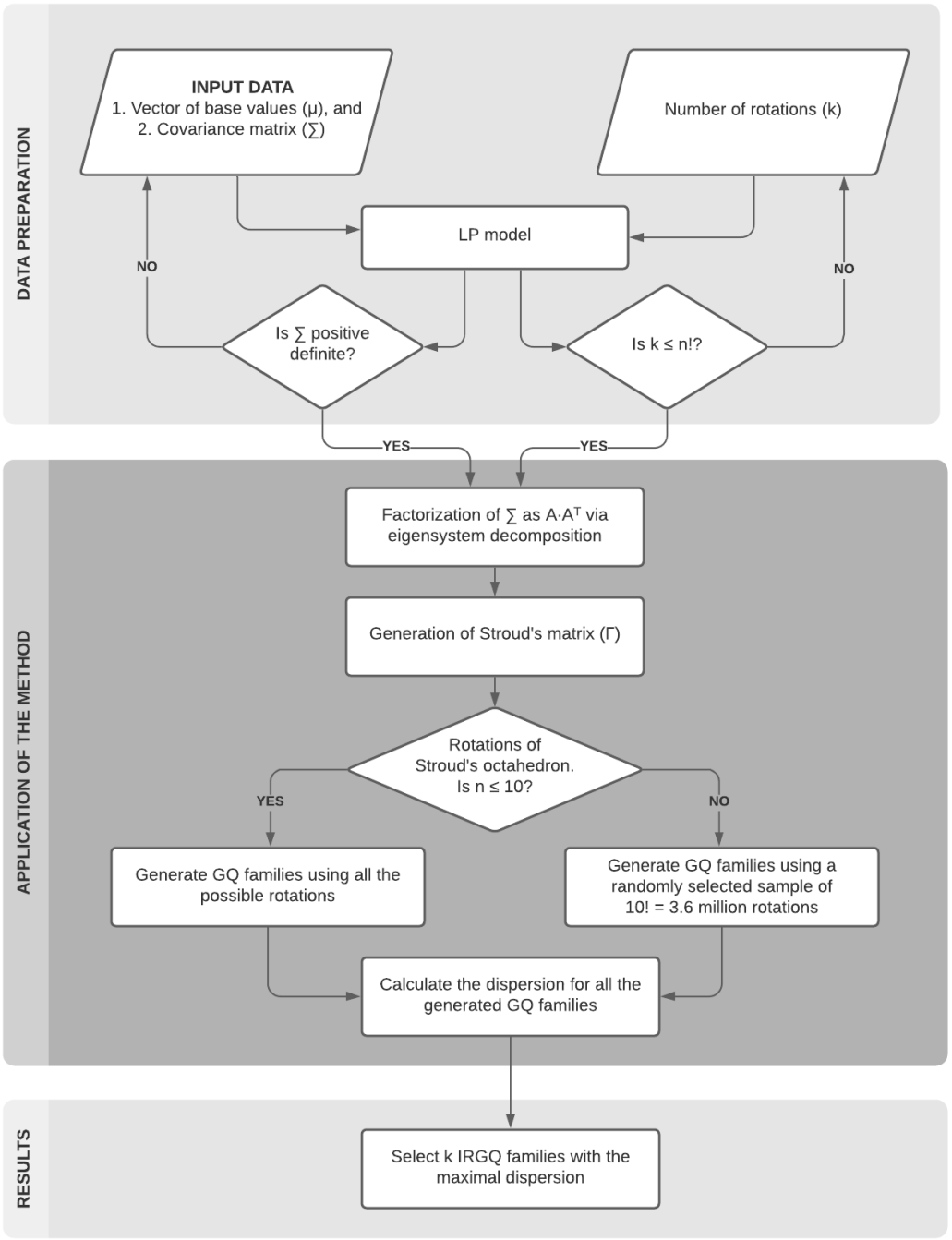

Figure 4.3. The process of identifying good rotations.

Let us consider a simple three-dimensional example with the following randomly generated covariance matrix Σ and vector of base values $\vec{\mu}$:

$$\mu = \begin{bmatrix} 1.43459 \\ 9.24601 \\ 6.47543 \end{bmatrix} \text{ and } \Sigma = \begin{bmatrix} 0.707855 & 0.361825 & -0.242114 \\ 0.361825 & 0.316408 & -0.226077 \\ -0.242114 & -0.226077 & 0.450200 \end{bmatrix}.$$

From equations (4.9) – (4.11), we obtain the following matrix with Stroud points:

$$\Gamma = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\sqrt{2} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \sqrt{2} \\ \sqrt{\frac{3}{2}} & \sqrt{\frac{3}{2}} & 0 & -\sqrt{\frac{3}{2}} & -\sqrt{\frac{3}{2}} & 0 \\ -1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix}.$$

Then, using the eigensystem decomposition method of the linear transformation, we obtain the square matrix A satisfying $\Sigma = AA^T$:

$$A = \begin{bmatrix} -0.780552 & 0.292832 & 0.113329 \\ -0.504474 & -0.012914 & -0.248491 \\ 0.47447 & 0.468007 & -0.077767 \end{bmatrix}.$$

As explained in Stepanyan et al. (2019b), the rotations of Stroud's octahedron can be obtained by multiplying A with a permutation matrix. Since we are dealing with a three-dimensional problem here, the number of all the possible permutations, and hence the number of possible permutation matrices, will be equal to 3! = 6. Those permutation matrices are:

$$P_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, P_3 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$P_4 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, P_5 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, P_6 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

By inserting these matrices into the following formula, six families of GQ points will be generated:

$$GQ_i = A \cdot P_i \cdot \Gamma + \mu \cdot (1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1). \tag{4.17}$$

This yields:

$$GQ_1 = \begin{bmatrix} 1.12797 & 2.45850 & 2.42513 & 1.74121 & 0.41069 & 0.44406 \\ 9.12197 & 9.33842 & 10.2079 & 9.37005 & 9.15360 & 8.28408 \\ 7.46189 & 6.63536 & 5.88220 & 5.48898 & 6.31551 & 7.06867 \end{bmatrix},$$

$$GQ_2 = \begin{bmatrix} 0.72863 & 2.41816 & 2.24563 & 2.14056 & 0.45103 & 0.62356 \\ 8.59787 & 9.28547 & 9.97236 & 9.89415 & 9.20655 & 8.51966 \\ 6.24768 & 6.51270 & 5.33643 & 6.70319 & 6.43817 & 7.61444 \end{bmatrix},$$

and so on.

For each of the GQ families, we compute the dispersion, *i.e.,* $disp(GQ_k) = min\{\|x_j - x_l\| : 1 \le j \le l \le 6\}$. This yields the following values.

GQ_1	**GQ_2**	**GQ_3**	**GQ_4**	**GQ_5**	**GQ_6**
1.15083	0.69558	0.96563	0.69558	1.17519	0.90570

Since GQ_5 has the largest dispersion, it is the family that is chosen:

$$IRGQ = GQ_5$$

$$= \begin{bmatrix} 0.265921 & 0.691313 & 0.98149 & 2.60327 & 2.17787 & 1.88770 \\ 8.465360 & 8.790950 & 9.61034 & 10.0267 & 9.70107 & 8.88168 \\ 6.533540 & 7.579540 & 6.11741 & 6.41733 & 5.37133 & 6.83346 \end{bmatrix}.$$

4.7. Results

The quality of the results obtained by different GQ families from the ESIM model is evaluated against the estimated benchmarks computed by Artavia et al. (2015) using an MC-based method with a sample size of 4,000. The quality of individual variables is assessed using the percentage of deviations of the results from the benchmarks. In order to evaluate the quality of a rotation as a whole, we use the mean squared error (MSE) of the deviations for all variables.

Table 4.1 presents the percentage deviations of the individual results from the benchmarks and also the MSEs of these deviations for ten rotations with maximal dispersion and for ten rotations with minimal dispersion. The individual results obtained by the GQ families with maximal dispersion show that the deviations of the variables barley, rapeseed, and wheat variables range from approximately -4% to 2%, 0% to 1.5%, and -3% to 3%, respectively. On the other hand, the deviations of the results obtained by the GQ families with minimal dispersion for the same variables range from approximately -9.4% to 13.5%, -2.4% to 3%, and -9% to 3%, respectively. We notice that the ranges of the deviations of the MSEs are much larger in the group of the results approximated by the GQ families with minimal dispersion. More specifically, the standard deviations of the MSEs from the group with minimal dispersion exceed the standard deviations of the MSEs from the group with maximal dispersion by a factor of 7. While some of the GQ families with minimal dispersion have a very high MSE, others may perform relatively well. For example, the MSE of the results approximated by the GQ family MIN1 falls within the range of the MSEs obtained by the GQ families with maximal dispersion.

Table 4.1. Percentage deviations of the CVs of producer prices in the "Rest of the World" from the benchmarks and the MSEs of the deviations for each rotation. MAX1 – MAX10 denote the respective results obtained from the ten GQ families with maximal dispersion.

	Barley	Rapeseed	Wheat	MSE		Barley	Rapeseed	Wheat	MSE
MAX1	1.388	0.133	-0.799	0.861	MIN1	3.672	2.832	-1.627	8.050
MAX2	-3.340	0.405	-2.654	6.120	MIN2	-3.508	0.790	-4.305	10.490
MAX3	-4.052	0.855	-3.103	8.928	MIN3	-3.885	0.161	-6.760	20.272
MAX4	2.058	1.523	3.163	5.520	MIN4	-5.283	0.414	-1.956	10.637
MAX5	-3.573	0.806	-2.097	5.938	MIN5	-9.431	1.245	-8.638	55.034
MAX6	1.109	0.811	-0.262	0.652	MIN6	5.387	0.931	0.685	10.117
MAX7	-3.416	0.745	-0.310	4.107	MIN7	-5.034	1.592	2.686	11.695
MAX8	-3.773	0.069	-1.987	6.064	MIN8	13.512	0.582	-2.776	63.539
MAX9	-3.909	0.035	-2.937	7.970	MIN9	-4.608	-0.572	-3.337	10.899
MAX10	0.183	0.818	-2.245	1.914	MIN10	-5.607	-2.424	-8.037	33.972

Figure 4.4 presents the MSEs of the results for barley, rapeseed, and wheat obtained by each individual rotation, *i.e.*, ten rotations with maximal dispersion and ten rotations with minimal dispersion. The horizontal line is the average of the MSEs of the ten rotations. The average of the MSEs of the results obtained by the GQ families with maximal dispersion is 4.8%. The MSEs of these individual rotations range from approximately 1% to 9%. The average of the MSEs of the results obtained by the GQ families with minimal dispersion, in contrast, is 23.5% and thus fivefold higher. The MSEs obtained by the individual rotations of this group of results range from approximately 8% to 64%.

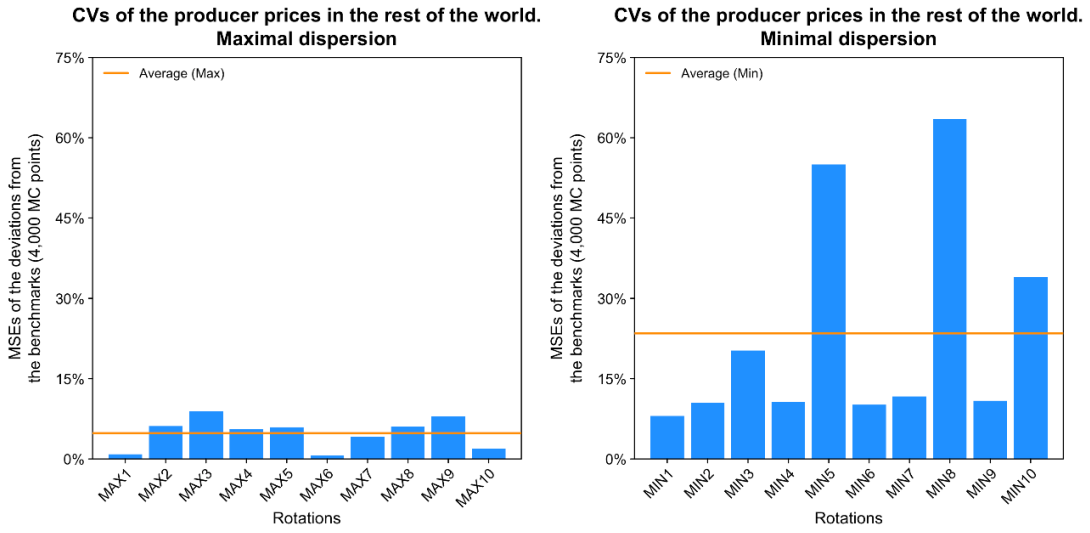

Figure 4.4. MSEs of the CVs of the producer prices in the rest of the world expressed as percentage deviations from the benchmarks in the ESIM model. MAX1 – MAX10 denote the results obtained by the ten GQ families with maximal dispersion, and MIN1 – MIN10 denote the results obtained by the ten GQ families with minimal dispersion.

The proposed method has been tested in two other economic simulation models, explained in Section 4.6.3, using the same experimental design.

Given the recursive-dynamic nature of the CGE model, the quality evaluation of the results obtained by individual rotations is measured as MSEs of percentage deviations of the mean absolute CVs of the growth rates of the production quantities from the benchmark (Figure 5). As shown in Figure 4.5, the magnitude of the MSEs in this model is much higher due to the recursive-dynamic structure of the model, the higher number of stochastic parameters included in the calculation of the MSEs and the cumulative effect of the deviations accumulated from the previous time periods. The difference between the average MSEs, shown by the horizontal lines, of the two groups of GQ points is approximately 4-fold. Meanwhile, the MSEs of the results using the individual rotations in the group with maximal dispersion of points ranged from 40 % to 92%. However, in the group with minimal dispersion, the MSEs ranged from 162% to 402%.

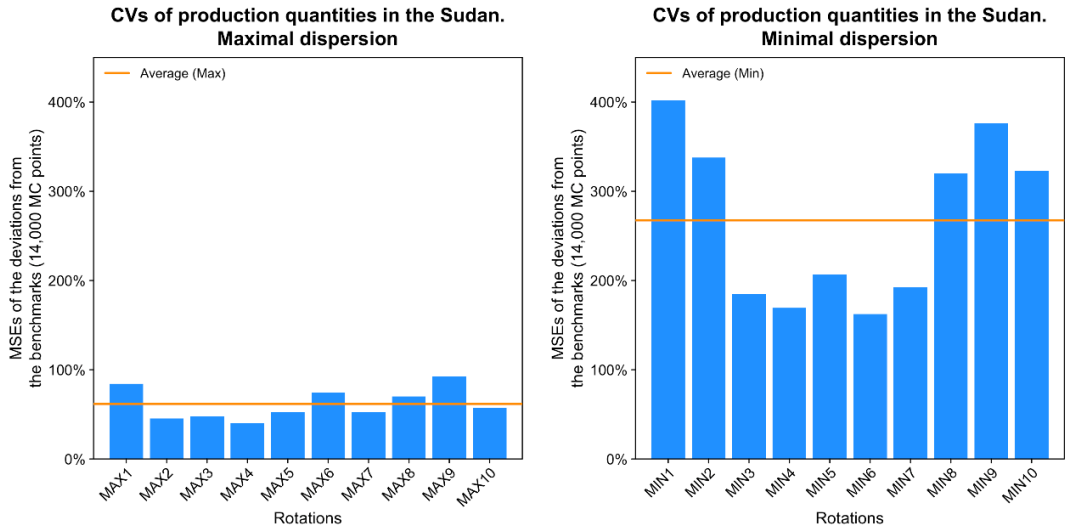

Figure 4.5. MSEs of the mean absolute CVs of the growth rates of production in the Sudan expressed as percentage deviations from the benchmarks in the recursive-dynamic CGE model. MAX1 – MAX10 denote the results obtained by the ten GQ families with maximal dispersion, and MIN1 – MIN10 denote the results obtained by the ten GQ families with minimal dispersion.

The results from the GLOBIOM model are again evaluated using the MSEs of the percentage deviations of the production quantities obtained by individual GQ rotations from the benchmarks for all stochastic variables. These results are presented in Figure 4.6. Similar to the results from the two previous models, one can observe that the range of the deviations of the results from the benchmarks obtained by the GQ points with maximal dispersion is much smaller than the range of those obtained by the GQ points with minimal dispersion. More specifically, the average of the MSEs obtained in the first group is less than half of that in the second group. The individual MSEs of the first group range from 7.6% to 16% whereas the MSEs in the second group range from 18.8% to 40.5%.

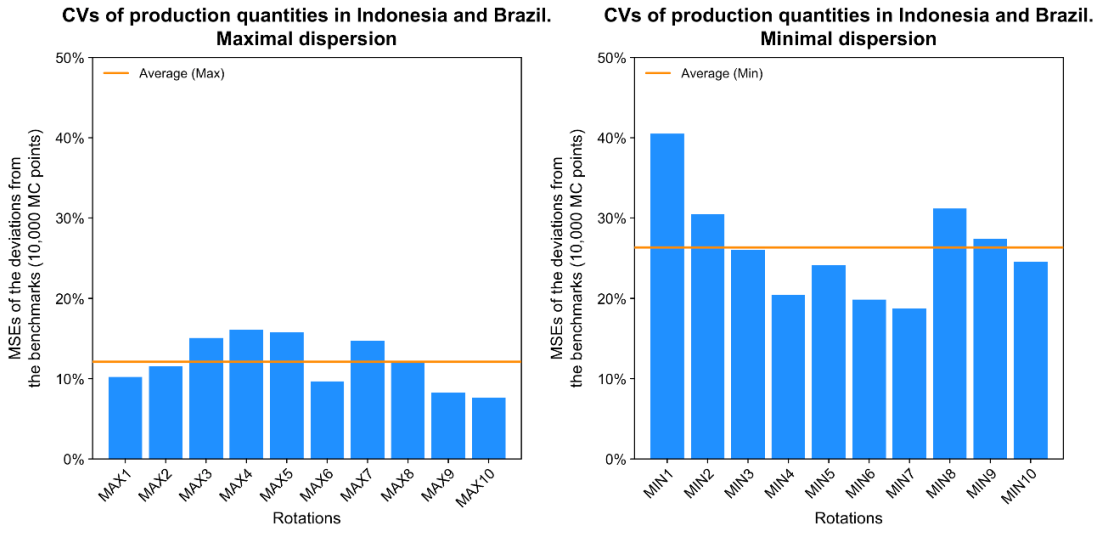

Figure 4.6. MSEs of the CVs of the production quantities in Indonesia and Brazil expressed as percentage deviations from the benchmarks in GLOBIOM. MAX1 – MAX10 denote the results obtained by the ten GQ families with maximal dispersion, and MIN1 – MIN10 denote the results obtained by the ten GQ families with minimal dispersion.

4.8. Discussion and conclusions

In this chapter, we address the questions posed by Artavia et al. (2015): Why do certain rotations of Stroud's octahedron generate GQ points that yield poor approximations of simulation model results, and how can rotations generating low approximation errors be chosen? These questions have remained open since the finding by Artavia et al. (2015) that the quality of the approximations by the GQ method is related to the rotations of Stroud's octahedron. This finding has also been confirmed by several other studies (Stepanyan et al. 2019a; Stepanyan et al. 2019b; Villoria and Preckel 2017). Our hypothesis for this study, based on extensive computations, was that the primary factor influencing the quality of approximations by the GQ method is the disposition of the GQ points generated by the permutations of the n coordinates of Stroud's n-octahedron. Hence, the rotations that generate GQ points lying close to each other (minimal dispersion) will supposedly produce poor quality results, and the rotations

generating GQ points lying far from each other (maximal dispersion) will produce high quality results. To test this hypothesis, we constructed a simple LP model, which is provided along with this article that is able to distinguish between good and bad quality rotations based on the criteria explained above. Using this LP model, we generated a sample of ten rotations from each group and tested them in the same simulation model as Artavia et al. (2015), *i.e.,* the ESIM model (Grethe 2012). In order to avoid biases caused by the specific simulation model and data, we also tested this hypothesis in two other simulation models, namely, a single-country recursive-dynamic CGE model (Diao and Thurlow 2012) and a global PE model (Havlík et al. 2011; Havlík et al. 2014). The results from all three models are similar. They show that on average, the GQ points with maximal dispersion produce results that are considerably closer to the benchmark than those with minimal dispersion. Since the quality of a rotation should be evaluated using the quality of the approximations of all stochastic variables, we choose the MSE of the stochastic variables from the benchmarks as a quality indicator.

Based on the empirical results from three different simulation models, we can safely claim that the disposition of the GQ points is an important factor determining the quality of approximations. Our findings are directly relevant for researchers applying large-scale simulation models who often struggle applying conventional stochastic modeling methods since they require thousands of iterations at a very high computational cost (Mary et al. 2018; Stepanyan et al. 2019b; Razavi et al. 2019; Gan et al. 2014). Our recommendation is thus to choose the GQ family with maximal dispersion. If an even better quality approximation and the avoidance of outliers are desired, the results could be further improved by combining our approach with the MRGQ method presented in Chapter 3. This would imply selecting more than one GQ family with a high dispersion and taking the average of the approximated results.

With our findings, we answer the open questions posed by Artavia et al. (2015) and address the concerns regarding the quality of approximated results when using the GQ method for stochastic modeling. With the growing size and scope of economic simulation models, efficient stochastic modeling methods are likely to become more popular since the conventional MC-based methods impose high computational and data management requirements.

While the introduced IRGQ method has a strong attraction for applied analysis due to its ability to improve the precision of the approximations via the GQ method using minimal computational requirements, open research questions remain to be addressed. Future research may generate a better understanding of other factors that influence the quality of approximations when applying the GQ method. These findings may contribute to understanding why GQ families with small dispersion sometimes produce results that are in the range of those produced by GQ families with high dispersion.

Chapter 5
Concluding remarks

Chapter 5

5. Concluding remarks

Given the fast growth of available computational capacities, simulation models are expanding in scope and levels of complexity. This expansion, however, also increases the uncertainty surrounding the results generated by such models. Therefore, uncertainty analysis is becoming an integral part of model development. The literature review presented in Chapter 3 reveals that MC-based methods are the most widely used approach when conducting uncertainty analyses in simulation models. Several factors can explain this situation.

First, they are easy to apply. Many modeling languages come with one of these approaches already integrated; thus, conducting uncertainty analyses is a matter of adding a line of code or pushing a button. Second, if applied correctly (*i.e.,* with consideration for correct sample sizes via convergence evaluations), such methods are very effective. In contrast, the application of efficient methods of uncertainty analyses in simulation modeling, such as the GQ method, is relatively new. In addition, their application requires additional effort, as they are not as widely integrated into the available software packages as MC-based approaches. Moreover, different researchers have shown evidence that the results approximated by the GQ method are not as precise as the ones obtained by MC-based methods. Therefore, this thesis, first and foremost, aims to improve the quality of efficient uncertainty analysis methods and second to reduce the barriers to their application by constructing two programming models that make the process of generating efficient points as simple as the process of generating MC points.

Section 5.1 presents the key findings of this thesis, while Section 5.2 discusses its limitations. Section 5.3 discusses options for future research.

5.1. Key findings

The following primary (1 and 2) and secondary (3–5) research objectives are addressed in this thesis:

1. Develop a method that reduces the approximation error in the GQ method to the level that would allow its application in large-scale simulation models without concerns regarding the quality of the approximated results.
2. Determine the factors influencing the quality of the approximations obtained by certain rotations of Stroud's octahedron.
3. Confirm, in a more comprehensive framework, the findings of Artavia et al. (2015) that the quality of the approximations produced by the GQ method is indeed influenced by the rotations of Stroud's octahedron.
4. Incorporate and test the method in other well-established, large-scale simulation models addressing agro-environmental issues.
5. Demonstrate the computational efforts required to obtain reliable results when applying probabilistic methods of stochastic analysis in large-scale simulation models.

The first and fifth research objectives are tackled in Chapter 3. In this chapter, a novel approximation error reduction method, named MRGQ, for Stroud's (1957) order 3 GQ has been developed. The proposed method has been successfully tested in three different large-scale simulation models: a comparative-static, single-country CGE model based on the STAGE model (McDonald and Thierfelder 2015) extended for, and applied to, Bhutan (Feuerbacher et al. 2018); GLOBIOM (Havlík et al. 2011; Havlík et

al. 2014), a global PE model developed for the agricultural and forestry sectors; and a multi-sector recursive-dynamic CGE model (Diao and Thurlow 2012) extended for the Sudan by Siddig et al. (2020). To evaluate the quality of the developed method, benchmark results for each model have been generated using a probabilistic method known as LHS with converged sample sizes, following the method suggested by Yang (2011).

The results obtained from all three models reveal two distinct advantages of the proposed method. First, the MRGQ method requires a considerably smaller number of iterations for stochastic analysis than the LHS method. More specifically, the MRGQ method reduces the number of iterations by more than 90% in all three models, thus reducing the required computational costs for conducting stochastic analyses to an extent that allows such analyses to be carried out on a single standard notebook. Second, using only a fraction of the required computational resources, the MRGQ method produces high-quality results comparable to the results obtained by the computationally expensive MC-based methods. In addition, a publicly available programming model is formulated that, given the necessary input data, generates MRGQ points that can then be incorporated into any simulation model for stochastic analyses. These findings are highly relevant for applied modelers. Essentially, the MRGQ does not force them to choose between computational efforts and the quality of the model results, unlike the probabilistic approaches. Furthermore, the method also avoids the chance of obtaining low-quality approximation when applying a single GQ.

The second research objective is addressed in Chapter 4, along with the second methodological novelty of this thesis. Using the empirical evidence obtained from three large-scale simulation models, it is demonstrated that the dispersion of the GQ points is an important determinant of the quality of the approximations. These results also

allow us to address the questions posed by Artavia et al. (2015): Why do certain rotations of Stroud's octahedron generate GQ points that yield poor approximations of simulation model results? How can rotations generating low approximation errors be chosen? Subsequently, the second methodological novelty of this study is developed. The IRGQ method performs all possible rotations of Stroud's generalized n-octahedron by permuting the n coordinates and selects the rotations that produce GQ points with the largest dispersions. An LP model is constructed that, given the input data, generates IRGQ points that can be applied to any simulation model for stochastic analyses. The results from ESIM (Grethe 2012), GLOBIOM (Havlík et al. 2011; Havlík et al. 2014), and the recursive-dynamic CGE model (Diao and Thurlow 2012) show that using GQ points generated from only one rotation of the IRGQ method can produce good-quality results. Furthermore, it can be combined with the MRGQ method to generate results with even higher precision.

Objectives 3 and 4 are fulfilled in Chapters 3 and 4. In Chapter 3, several randomly generated GQ rotations are tested in three well-established, large-scale simulation models, thus overcoming the limitation of the approach of Artavia et al. (2015), who selected the rotations to be tested in an *ad hoc* way. The test has established that, depending on the rotation, the quality of the approximation produced by the GQ method varies considerably. The results from Chapter 4 demonstrate a similar picture, although the rotations presented in this chapter are not generated randomly. Overall, the developed methods are tested in four simulation models addressing agro-environmental issues: a comparative-static, single-country CGE model, the global PE model GLOBIOM of the agricultural and forestry sectors; a multi-sector recursive-dynamic CGE model and a global PE model called ESIM.

5.2. Limitations of the thesis

Although the proposed novel methods in this thesis demonstrate very promising results based on four large-scale simulation models, certain limitations should be addressed.

First, as demonstrated in Chapter 3, the points generated by the proposed GQ-based methods are restricted in their variation around the mean on each coordinate axis, which restricts their ability to capture the extreme tails (*i.e.,* rare occurrences) of their given probability distribution. This limitation can be crucial in certain fields of application, such as the impact of extreme weather events. As a remedy to this limitation, we could combine the methods proposed in this study with the broader GQ sampling method proposed by Preckel et al. (2011), which would allow a widening of the sampling intervals by a desired factor.

Second, the proposed methods are restricted to approximating symmetric probability distributions. However, these methods can be extended to depict asymmetric regions using the approach developed by DeVuyst and Preckel (2007).

In Chapter 4, we present one factor influencing the quality of the approximations achieved when applying the GQ method. However, as GQ families with small dispersions sometimes produce results in the range of those produced by GQ families with large dispersions, we suspect that there might be additional factors influencing the quality. We suspect that such a factor may in fact be the arrangement of variables with stronger correlations and higher importance for the model in the covariance matrix.

5.3. Future research agenda

Following the limitations listed in Section 5.2, future research could include testing the proposed approaches for capturing the tails of the distributions, as well as the asymmetric regions, in large-scale simulation models.

Another area of future research could involve exploring other factors influencing the quality of the approximations obtained when applying the GQ method. More specifically, one could analyze to what extent model specifications and constraints, such as price floors and ceilings and production quotas, limit the quality of the GQ method.

To further reduce the required computational efforts one could first identify the model variables/parameters that have a higher influence on the uncertainty of the model results and consider only those variables/parameters in the final stochastic analysis. This is especially relevant for the proposed methods because the number of required iterations of these methods directly depends on the number of stochastic variables/parameters considered in the model.

Finally, we encourage researchers to apply and test the proposed novel methods in other simulation models addressing practical research questions

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